Yasuda-Shedlovsky Result

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

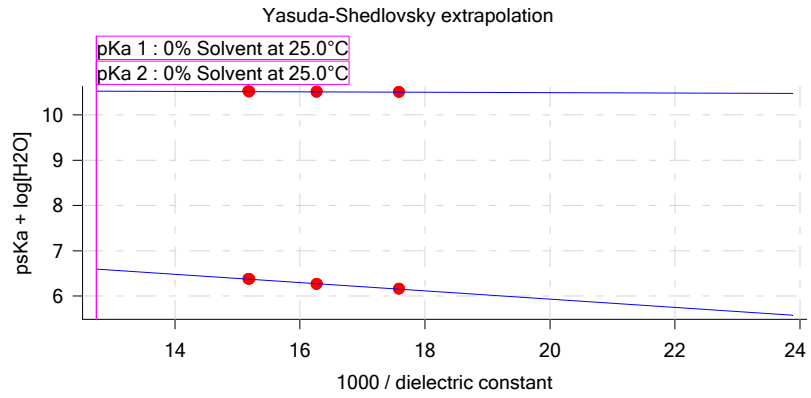
Yasuda-Shedlovsky result

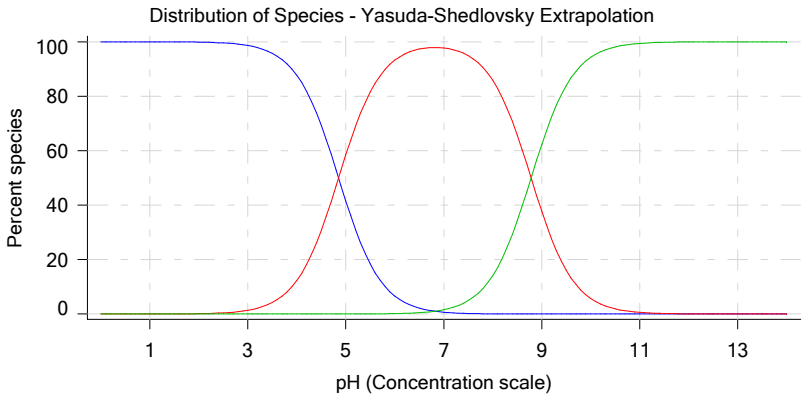
Extrapolation type	pKa 0%	SD	Intercept	Slope	R²	Ionic strength	Temperature
Yasuda-Shedlovsky	4.85	±0.01	7.76	-91.0605	0.9963	0.167 M	25.0°C
Yasuda-Shedlovsky	8.78	±0.01	10.59	-4.9077	0.4737	0.167 M	25.0°C

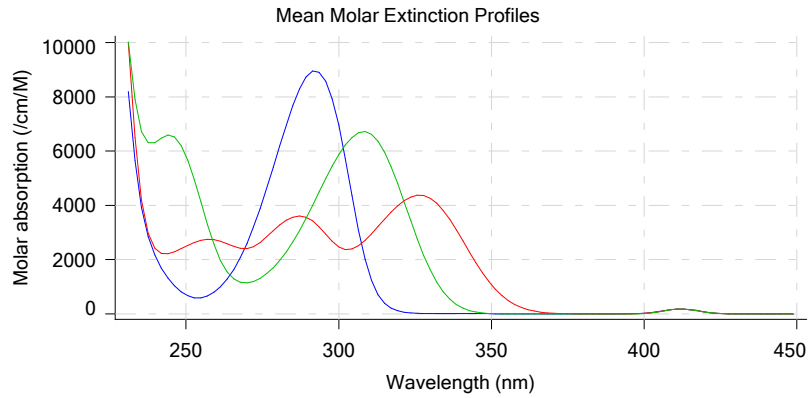
Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	psKa 2
18E-22011 Points 4 to 43	48.92 %	Up	UV-metric pKa	56.9	25.0 M	0.158 M	25.0°C ☑	4.76 ☑	9.11
18E-22011 Points 45 to 88	38.89 %	Up	UV-metric pKa	61.5	30.6 M	0.168 M	25.0°C ☑	4.78 ☑	9.02
18E-22011 Points 90 to 135	29.14 %	Up	UV-metric pKa	65.9	36.4 M	0.175 M	25.0°C ☑	4.82 ☑	8.96
18E-22012 Points 4 to 43	48.97 %	Up	UV-metric pKa	56.8	25.0 M	0.158 M	25.0°C ☑	4.76 ☑	9.10
18E-22012 Points 45 to 88	38.95 %	Up	UV-metric pKa	61.5	30.6 M	0.168 M	25.0°C ☑	4.78 ☑	9.01
18E-22012 Points 90 to 134	29.32 %	Up	UV-metric pKa	65.8	36.3 M	0.174 M	25.0°C ☑	4.82 ☑	8.96
18E-22013 Points 4 to 43	48.94 %	Up	UV-metric pKa	56.9	25.0 M	0.158 M	25.0°C ☑	4.76 ☑	9.11
18E-22013 Points 45 to 85	38.99 %	Up	UV-metric pKa	61.4	30.6 M	0.168 M	25.0°C ☑	4.79 ☑	9.03
18E-22013 Points 87 to 120	29.29 %	Up	UV-metric pKa	65.8	36.3 M	0.175 M	25.0°C ☑	4.82 ☑	8.95

Graphs







Multiset assays

Assay 1 of 3

Sample name	UV-metric psKa_0417936-0002
Assay name	UV-metric psKa
Assay ID	18E-22011
Instrument ID	T311053
Imported from	C:\Sirius_T3\18E-22011_Pyridoxine HCl_UV-metric psKa_0417936-0002.t3r
Imported on	5/22/2018 4:17:18 PM
Analyst name	Dorothy Levorse
Experiment start time	5/22/2018 12:19:28 PM

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Multiset assays (continued)

Assay 2 of 3

Sample name	UV-metric psKa_0417936-0002
Assay name	UV-metric psKa
Assay ID	18E-22012
Instrument ID	T311053
Imported from	C:\Sirius_T3\18E-22012_Pyridoxine HCl_UV-metric psKa_0417936-0002.t3r
Imported on	5/22/2018 4:17:18 PM
Analyst name	Dorothy Levorse
Experiment start time	5/22/2018 1:35:32 PM

Assay 3 of 3

Sample name	UV-metric psKa_0417936-0002
Assay name	UV-metric psKa
Assay ID	18E-22013
Instrument ID	T311053
Imported from	C:\Sirius_T3\18E-22013_Pyridoxine HCl_UV-metric psKa_0417936-0002.t3r
Imported on	5/22/2018 4:17:18 PM
Analyst name	Dorothy Levorse
Experiment start time	5/22/2018 2:50:50 PM

UV-metric psKa_0417936-0002 Titration 1 of 3 18E-22011 Points 4 to 43

Results

pKa 1	**4.76**
pKa 2	**9.11**
RMSD	**0.037 0.030 0.024**
Chi squared	**0.1587**
PCA calculated number of pKas	**4**
Average ionic strength	**0.158 M**
Average temperature	**25.0°C**
Analyte concentration range	**60.6 µM to 56.8 µM**
Methanol weight %	**48.9 %**
Dielectric constant	**56.9**
Water concentration	**25.0 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.455 to 12.545**

Warnings and errors

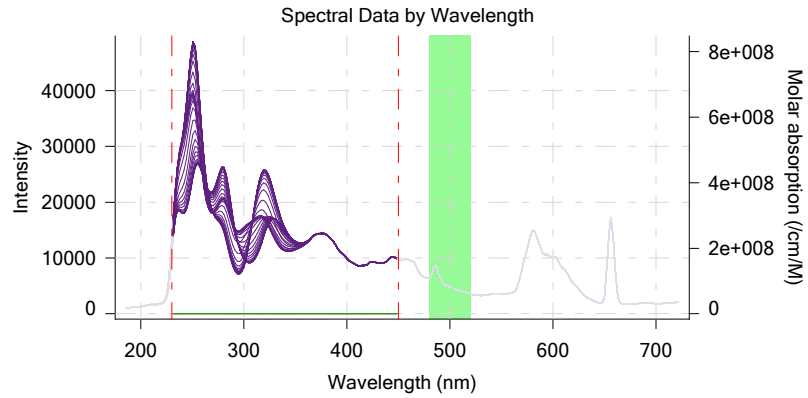
Errors	None
Warnings	PCA calculation disagrees with predicted number of pKas

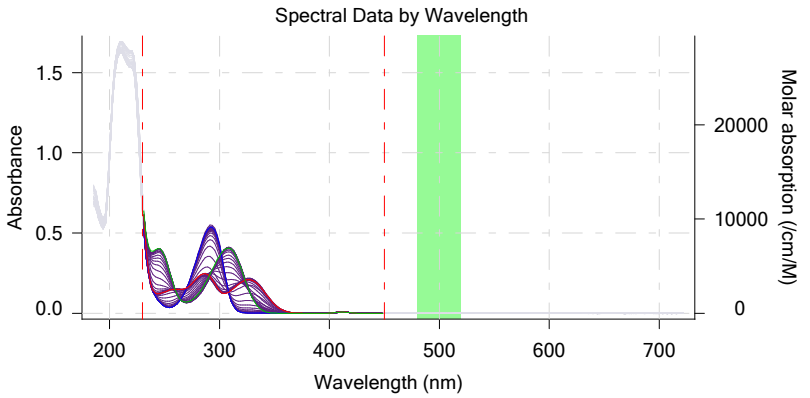
Assay Settings

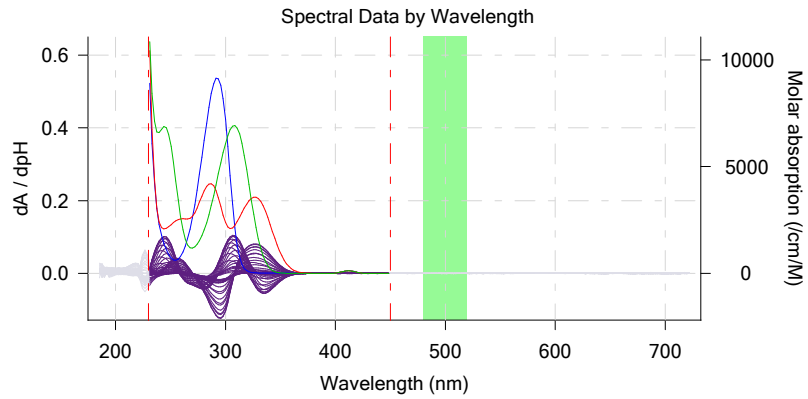
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

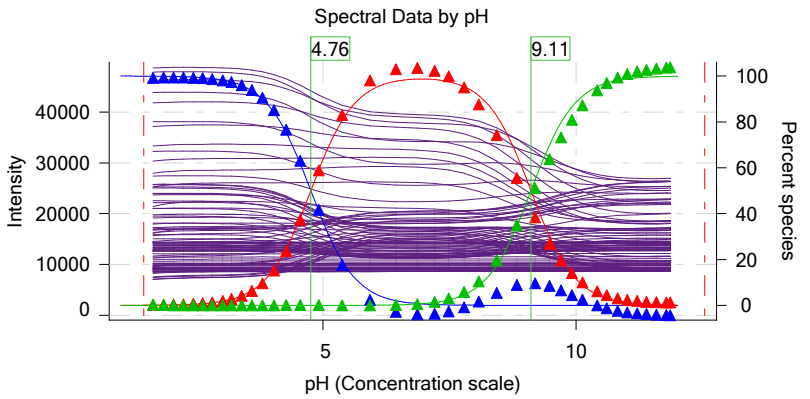
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

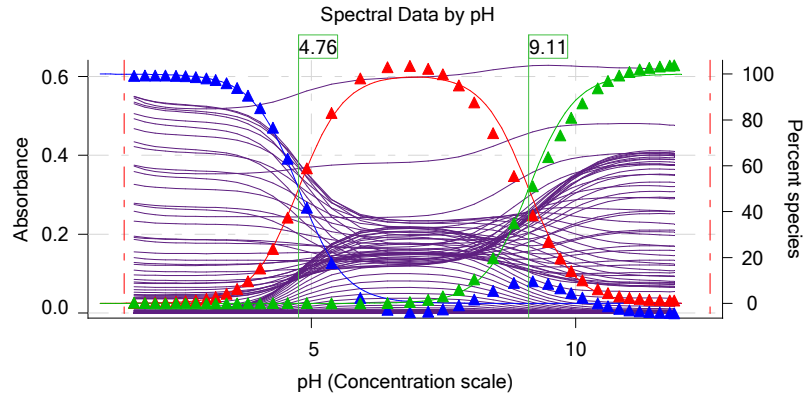
Graphs

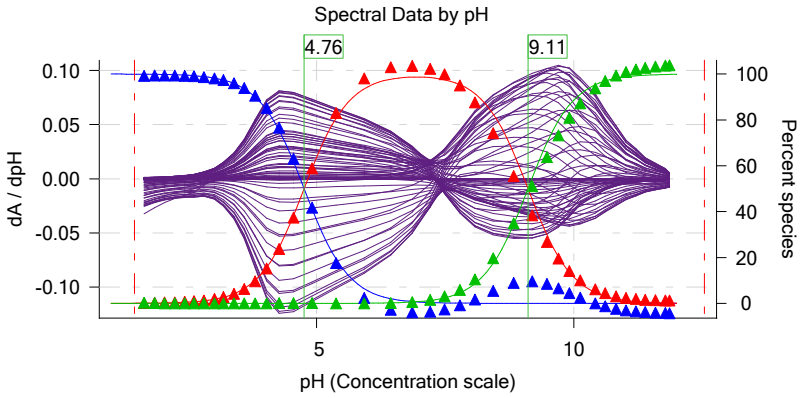


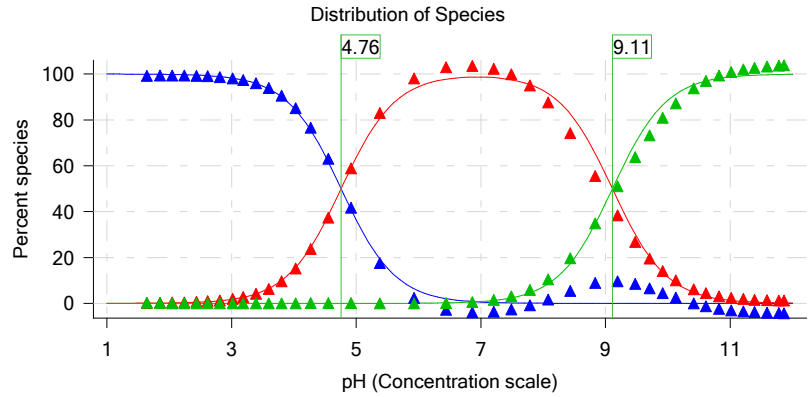


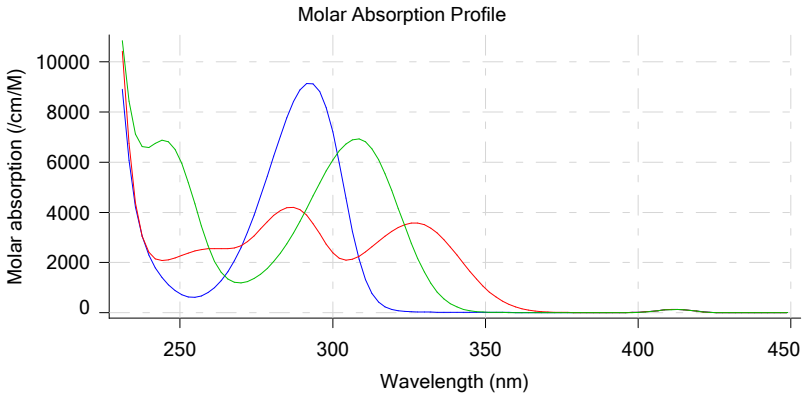






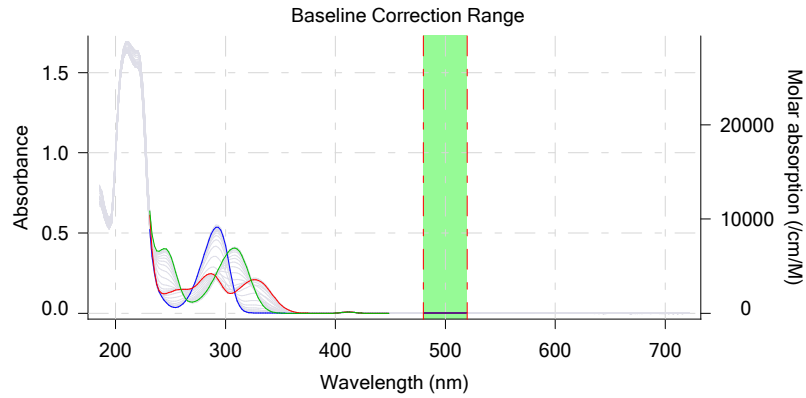


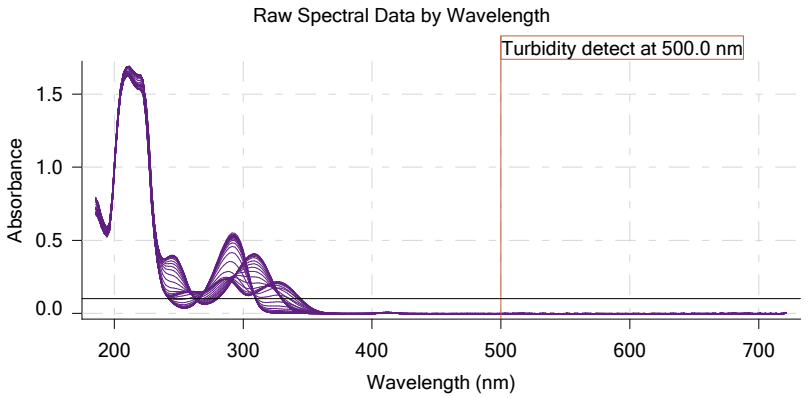




Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Graphs (continued)





UV-metric psKa_0417936-0002 Titration 2 of 3 18E-22011 Points 45 to 88

Results

pKa 1	**4.78**
pKa 2	**9.02**
RMSD	**0.045 0.033 0.031**
Chi squared	**0.2321**
PCA calculated number of pKas	**3**
Average ionic strength	**0.168 M**
Average temperature	**25.0°C**
Analyte concentration range	**49.2 µM to 46.1 µM**
Methanol weight %	**38.9 %**
Dielectric constant	**61.5**
Water concentration	**30.6 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.471 to 12.547**

Warnings and errors

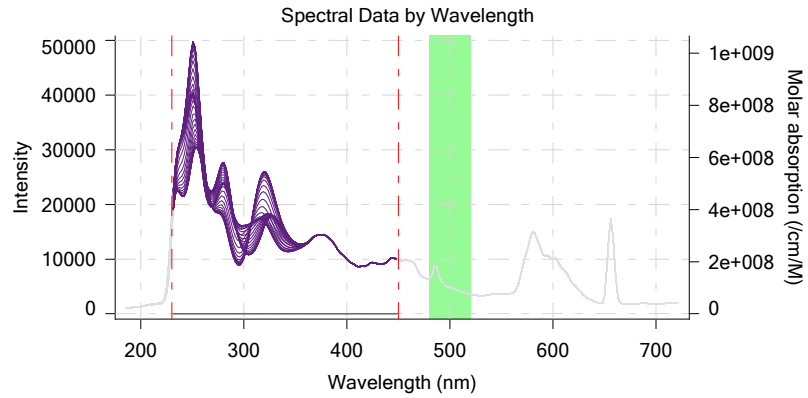
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

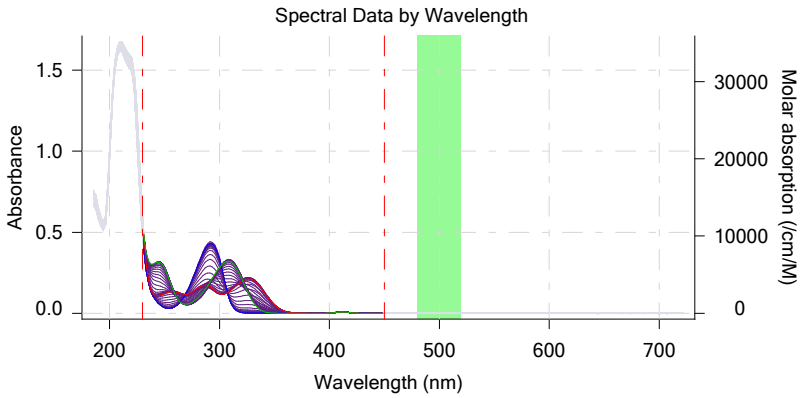
Assay Settings

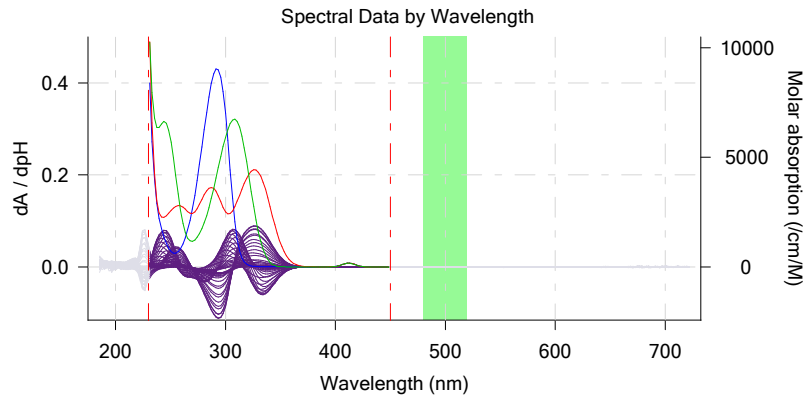
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

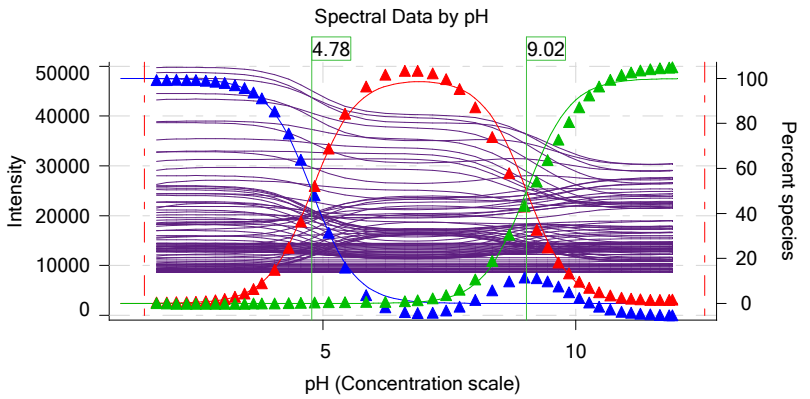
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

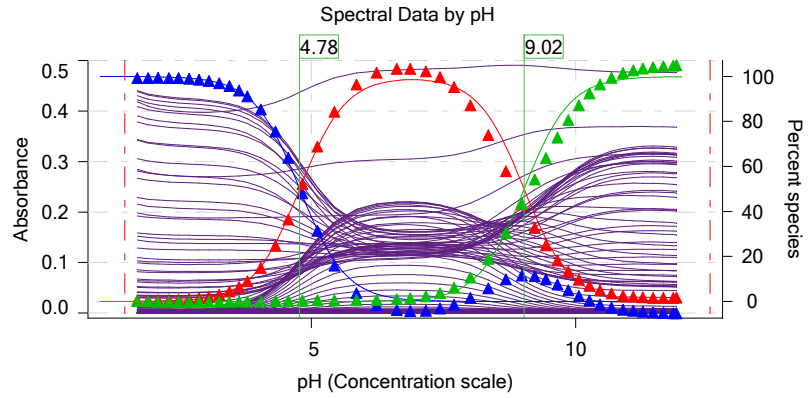
Graphs

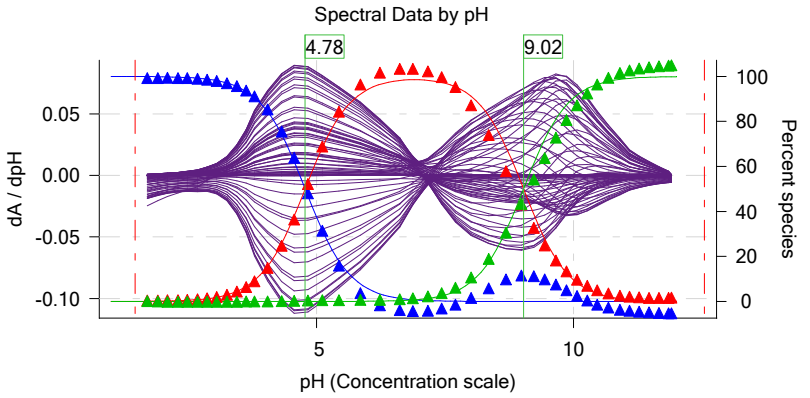


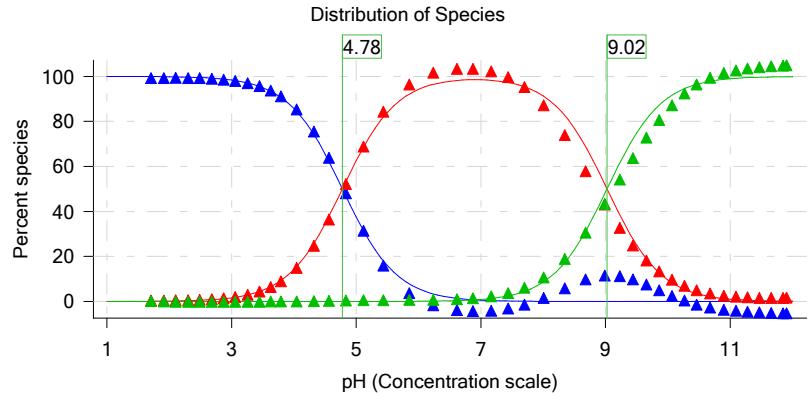


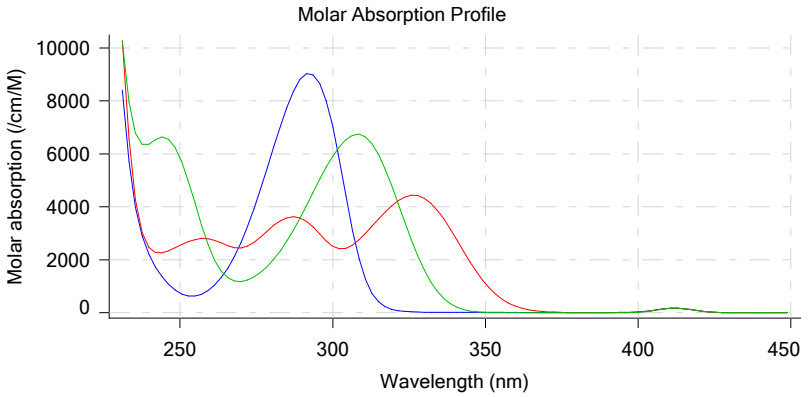






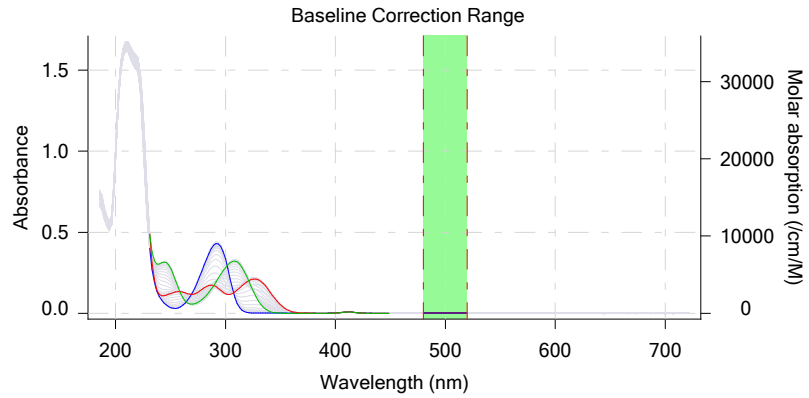


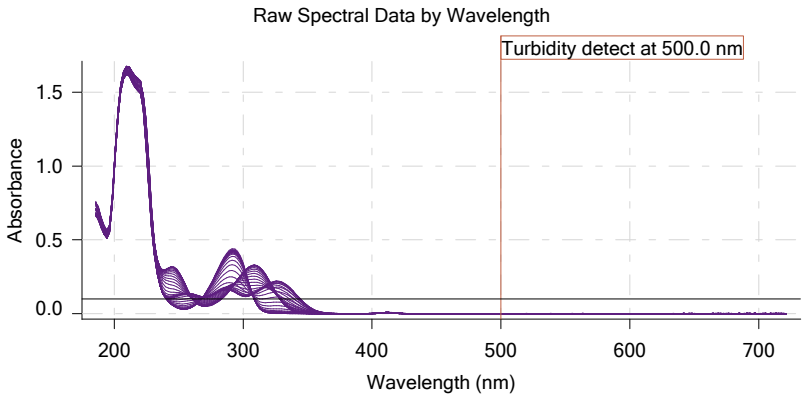




Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Graphs (continued)





UV-metric psKa_0417936-0002 Titration 3 of 3 18E-22011 Points 90 to 135

Results

pKa 1	**4.82**
pKa 2	**8.96**
RMSD	**0.046 0.031 0.036**
Chi squared	**0.2797**
PCA calculated number of pKas	**3**
Average ionic strength	**0.175 M**
Average temperature	**25.0°C**
Analyte concentration range	**37.6 µM to 35.3 µM**
Methanol weight %	**29.1 %**
Dielectric constant	**65.9**
Water concentration	**36.4 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.487 to 12.546**

Warnings and errors

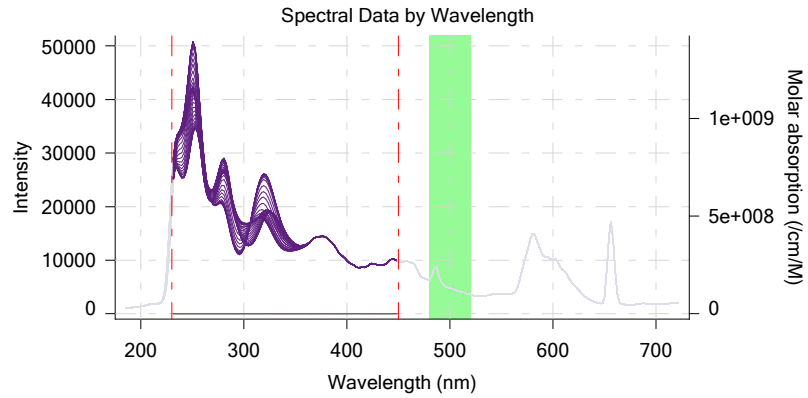
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

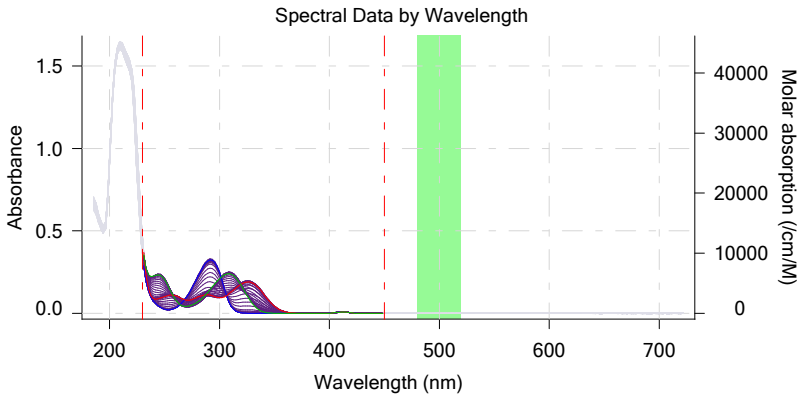
Assay Settings

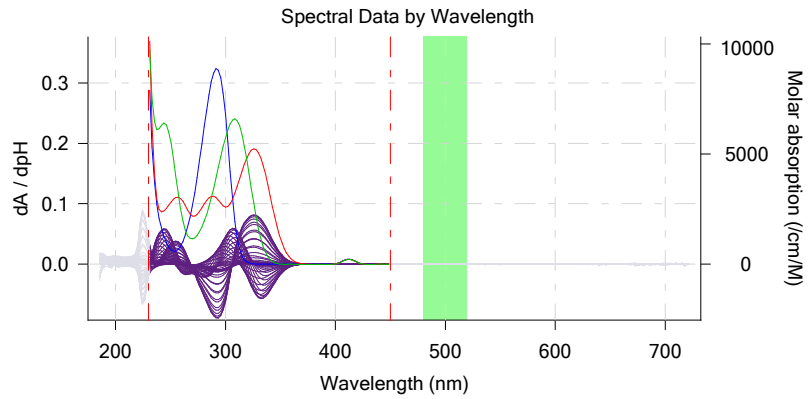
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

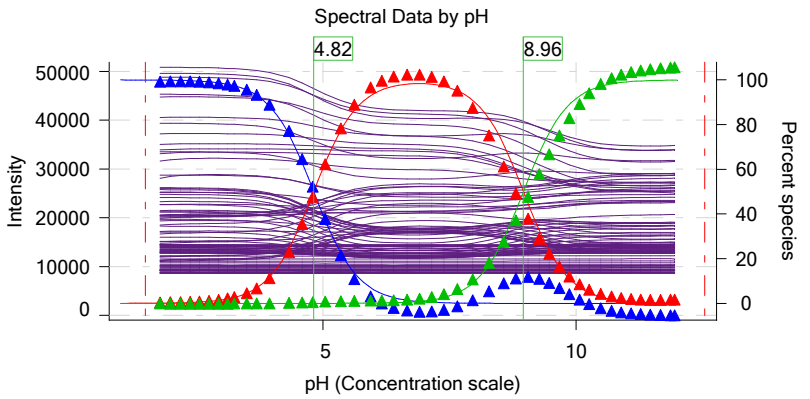
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

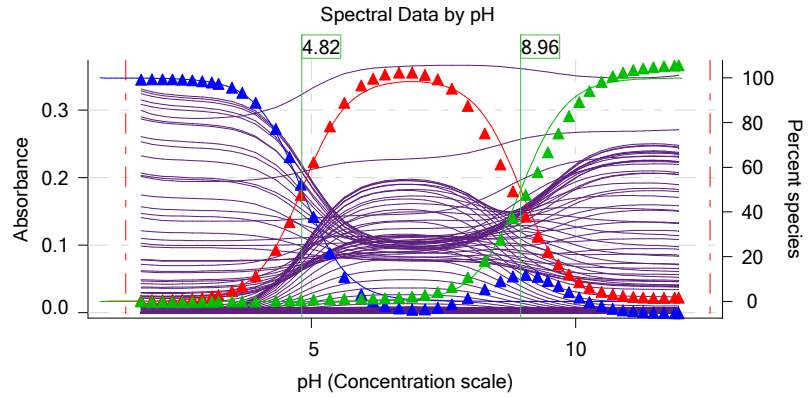
Graphs

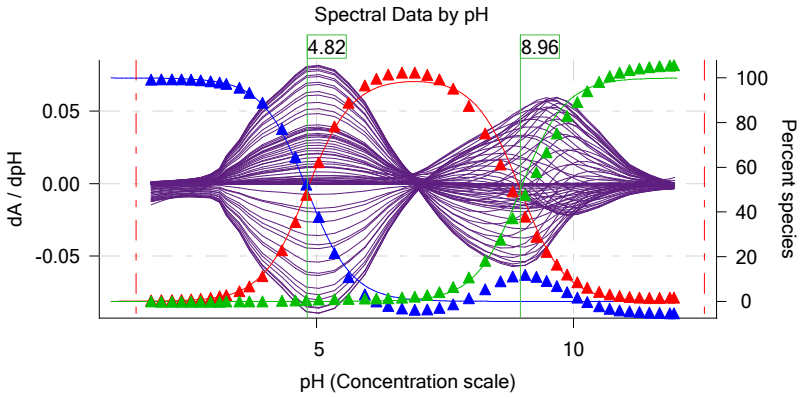


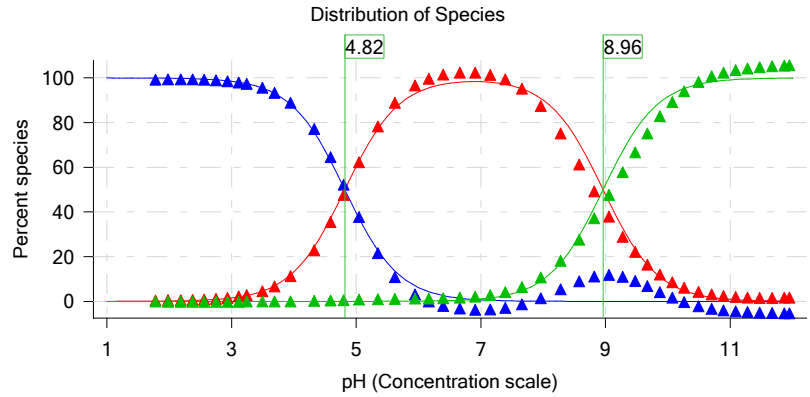


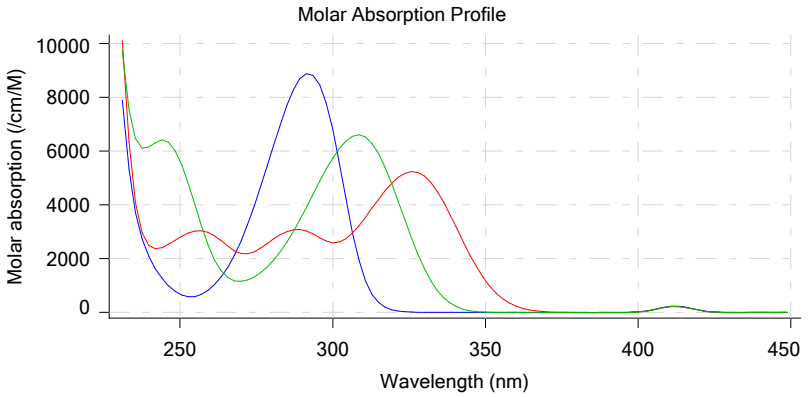






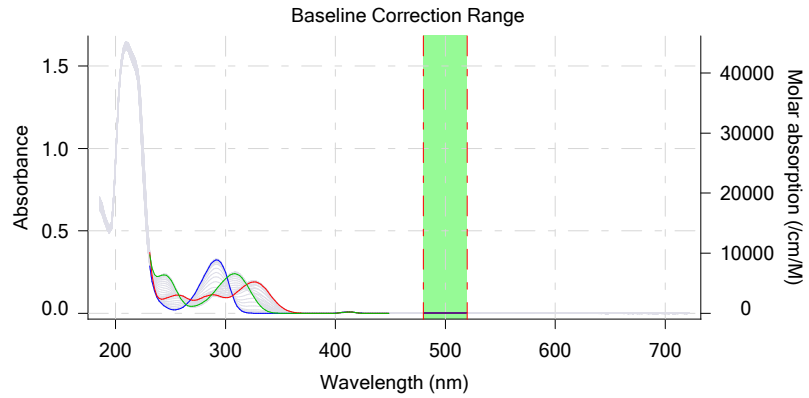


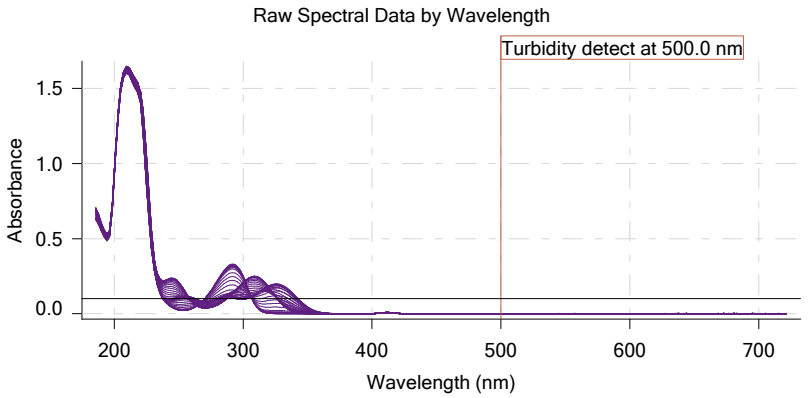




Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Graphs (continued)





UV-metric psKa_0417936-0002 18E-22011 Assay 1 of 3

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	Pyridoxine HCl	5/22/2018 9:07:27 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	5/22/2018 9:07:27 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.048630 M	5/22/2018 9:07:27 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	205.64	5/22/2018 9:07:35 AM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	5/22/2018 9:07:27 AM	User entered value
Sample is a	Ampholyte	5/22/2018 9:07:27 AM	User entered value
pKa 1	4.90	5/22/2018 9:07:27 AM	User entered value
Type	Base	5/22/2018 9:07:27 AM	User entered value
pKa 2	8.80	5/22/2018 9:07:27 AM	User entered value
Type	Acid	5/22/2018 9:07:27 AM	User entered value
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	5/22/2018 9:07:27 AM	User entered value
logP (X -)	-10.00		Default value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared
3:47.3	Dark spectrum								
3:48.9	Reference spectrum								
4:16.5	Volume reset due to vial change								
5:00.7	Initial pH = 7.87								
6:10.4	Data point 4	0.34995 mL	0.07726 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.955	-0.00772	0.61965
6:39.5	Data point 5	0.34995 mL	0.07726 mL	0.02813 mL	1.15005 mL	0.02500 mL	2.156	0.01115	0.56590
6:56.5	Data point 6	0.34995 mL	0.07726 mL	0.04501 mL	1.15005 mL	0.02500 mL	2.347	0.01384	0.57080
7:13.4	Data point 7	0.34995 mL	0.07726 mL	0.05588 mL	1.15005 mL	0.02500 mL	2.538	0.03397	0.85354
7:30.4	Data point 8	0.34995 mL	0.07726 mL	0.06284 mL	1.15005 mL	0.02500 mL	2.730	0.00492	0.31739
7:47.2	Data point 9	0.34995 mL	0.07726 mL	0.06733 mL	1.15005 mL	0.02500 mL	2.909	0.01020	0.66043
8:04.0	Data point 10	0.34995 mL	0.07726 mL	0.07030 mL	1.15005 mL	0.02500 mL	3.100	0.00803	0.74619
8:20.8	Data point 11	0.34995 mL	0.07726 mL	0.07220 mL	1.15005 mL	0.02500 mL	3.302	0.01901	0.96883
8:37.4	Data point 12	0.34995 mL	0.07726 mL	0.07338 mL	1.15005 mL	0.02500 mL	3.472	0.01793	0.88521
9:09.6	Data point 13	0.34995 mL	0.07726 mL	0.07441 mL	1.15005 mL	0.02500 mL	3.675	0.02585	0.91199

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
9:41.6	Data point 14	0.34995 mL	0.07726 mL	0.07505 mL	1.15005 mL	0.02500 mL	3.875	0.03952	0.97762	0.00
10:13.5	Data point 15	0.34995 mL	0.07726 mL	0.07549 mL	1.15005 mL	0.02500 mL	4.079	0.06259	0.96397	0.00
10:45.4	Data point 16	0.34995 mL	0.07726 mL	0.07603 mL	1.15005 mL	0.02500 mL	4.303	0.09345	0.99322	0.00
11:12.3	Data point 17	0.34995 mL	0.07726 mL	0.07627 mL	1.15005 mL	0.02500 mL	4.542	0.09632	0.98024	0.00
11:45.3	Data point 18	0.34995 mL	0.07726 mL	0.07653 mL	1.15005 mL	0.02500 mL	4.821	0.09636	0.97545	0.00
12:30.6	Data point 19	0.34995 mL	0.07726 mL	0.07667 mL	1.15005 mL	0.02500 mL	5.179	0.10014	0.99170	0.00
13:24.5	Data point 20	0.34995 mL	0.07726 mL	0.07679 mL	1.15005 mL	0.02500 mL	5.640	0.09945	0.99235	0.00
14:25.9	Data point 21	0.34995 mL	0.07726 mL	0.07688 mL	1.15005 mL	0.02500 mL	6.180	0.09930	0.99643	0.00
15:31.4	Data point 22	0.34995 mL	0.07726 mL	0.07698 mL	1.15005 mL	0.02500 mL	6.688	0.09832	0.99128	0.00
16:31.4	Data point 23	0.34995 mL	0.07726 mL	0.07709 mL	1.15005 mL	0.02500 mL	7.105	0.10060	0.99438	0.00
17:26.5	Data point 24	0.34995 mL	0.07726 mL	0.07723 mL	1.15005 mL	0.02500 mL	7.449	0.09811	0.98753	0.00
18:12.5	Data point 25	0.34995 mL	0.07726 mL	0.07738 mL	1.15005 mL	0.02500 mL	7.724	0.09986	0.98919	0.00
18:56.5	Data point 26	0.34995 mL	0.07726 mL	0.07754 mL	1.15005 mL	0.02500 mL	8.022	0.09930	0.98558	0.00
19:40.9	Data point 27	0.34995 mL	0.07726 mL	0.07768 mL	1.15005 mL	0.02500 mL	8.309	0.10075	0.99207	0.00
20:26.5	Data point 28	0.34995 mL	0.07726 mL	0.07782 mL	1.15005 mL	0.02500 mL	8.661	0.09753	0.98421	0.00
21:15.0	Data point 29	0.34995 mL	0.07726 mL	0.07796 mL	1.15005 mL	0.02500 mL	9.054	0.09457	0.97636	0.00
21:57.5	Data point 30	0.34995 mL	0.07726 mL	0.07810 mL	1.15005 mL	0.02500 mL	9.409	0.09700	0.98144	0.00
22:37.4	Data point 31	0.34995 mL	0.07726 mL	0.07825 mL	1.15005 mL	0.02500 mL	9.692	0.09580	0.98449	0.00
23:12.3	Data point 32	0.34995 mL	0.07726 mL	0.07839 mL	1.15005 mL	0.02500 mL	9.918	0.09682	0.98787	0.00
23:36.1	Data point 33	0.34995 mL	0.07726 mL	0.07855 mL	1.15005 mL	0.02500 mL	10.127	0.09847	0.96215	0.00
24:03.1	Data point 34	0.34995 mL	0.07726 mL	0.07879 mL	1.15005 mL	0.02500 mL	10.335	0.04977	0.96309	0.00
24:19.8	Data point 35	0.34995 mL	0.07726 mL	0.07912 mL	1.15005 mL	0.02500 mL	10.622	0.02210	0.94983	0.00
24:46.8	Data point 36	0.34995 mL	0.07726 mL	0.07966 mL	1.15005 mL	0.02500 mL	10.813	0.01386	0.91643	0.00
25:03.4	Data point 37	0.34995 mL	0.07726 mL	0.08062 mL	1.15005 mL	0.02500 mL	11.022	0.01074	0.92675	0.00
25:20.1	Data point 38	0.34995 mL	0.07726 mL	0.08215 mL	1.15005 mL	0.02500 mL	11.212	0.00860	0.60600	0.00
25:36.8	Data point 39	0.34995 mL	0.07726 mL	0.08452 mL	1.15005 mL	0.02500 mL	11.403	0.00392	0.54350	0.00
25:53.7	Data point 40	0.34995 mL	0.07726 mL	0.08822 mL	1.15005 mL	0.02500 mL	11.584	0.00233	0.25391	0.00
26:10.4	Data point 41	0.34995 mL	0.07726 mL	0.09386 mL	1.15005 mL	0.02500 mL	11.779	0.00676	0.80315	0.00
26:27.3	Data point 42	0.34995 mL	0.07726 mL	0.10282 mL	1.15005 mL	0.02500 mL	11.967	0.00481	0.56597	0.00
26:44.2	Data point 43	0.34995 mL	0.07726 mL	0.10786 mL	1.15005 mL	0.02500 mL	12.045	0.00461	0.59794	0.00
28:26.5	Reference spectrum									
29:31.0	Data point 45	0.50000 mL	0.19334 mL	0.10788 mL	1.15005 mL	0.02500 mL	1.971	-0.10001	0.97843	0.00
30:00.9	Data point 46	0.50000 mL	0.19334 mL	0.14059 mL	1.15005 mL	0.02500 mL	2.168	0.00102	0.05316	0.00
30:17.9	Data point 47	0.50000 mL	0.19334 mL	0.15882 mL	1.15005 mL	0.02500 mL	2.352	0.01120	0.81812	0.00
30:35.0	Data point 48	0.50000 mL	0.19334 mL	0.17063 mL	1.15005 mL	0.02500 mL	2.550	0.00693	0.30426	0.00
30:51.9	Data point 49	0.50000 mL	0.19334 mL	0.17801 mL	1.15005 mL	0.02500 mL	2.729	0.00261	0.04275	0.00
31:08.8	Data point 50	0.50000 mL	0.19334 mL	0.18290 mL	1.15005 mL	0.02500 mL	2.926	0.01737	0.83620	0.00
31:25.5	Data point 51	0.50000 mL	0.19334 mL	0.18596 mL	1.15005 mL	0.02500 mL	3.110	0.01260	0.81884	0.00
31:42.3	Data point 52	0.50000 mL	0.19334 mL	0.18798 mL	1.15005 mL	0.02500 mL	3.296	0.00889	0.80694	0.00
31:59.0	Data point 53	0.50000 mL	0.19334 mL	0.18930 mL	1.15005 mL	0.02500 mL	3.491	0.01995	0.97079	0.00
32:15.7	Data point 54	0.50000 mL	0.19334 mL	0.19012 mL	1.15005 mL	0.02500 mL	3.679	0.01497	0.86623	0.00
32:32.4	Data point 55	0.50000 mL	0.19334 mL	0.19066 mL	1.15005 mL	0.02500 mL	3.859	0.03662	0.98535	0.00
32:49.0	Data point 56	0.50000 mL	0.19334 mL	0.19102 mL	1.15005 mL	0.02500 mL	4.020	0.03589	0.83279	0.00
33:10.8	Data point 57	0.50000 mL	0.19334 mL	0.19139 mL	1.15005 mL	0.02500 mL	4.271	0.06012	0.99357	0.00
33:32.7	Data point 58	0.50000 mL	0.19334 mL	0.19165 mL	1.15005 mL	0.02500 mL	4.543	0.08457	0.98921	0.00
33:54.5	Data point 59	0.50000 mL	0.19334 mL	0.19182 mL	1.15005 mL	0.02500 mL	4.783	0.09749	0.97508	0.00
34:31.9	Data point 60	0.50000 mL	0.19334 mL	0.19196 mL	1.15005 mL	0.02500 mL	5.051	0.09819	0.99229	0.00
35:08.3	Data point 61	0.50000 mL	0.19334 mL	0.19207 mL	1.15005 mL	0.02500 mL	5.330	0.09758	0.97956	0.00
35:50.2	Data point 62	0.50000 mL	0.19334 mL	0.19217 mL	1.15005 mL	0.02500 mL	5.649	0.09843	0.98652	0.00
36:35.6	Data point 63	0.50000 mL	0.19334 mL	0.19226 mL	1.15005 mL	0.02500 mL	6.059	0.10020	0.98033	0.00
37:22.4	Data point 64	0.50000 mL	0.19334 mL	0.19236 mL	1.15005 mL	0.02500 mL	6.440	0.09816	0.98715	0.00
38:15.9	Data point 65	0.50000 mL	0.19334 mL	0.19247 mL	1.15005 mL	0.02500 mL	6.818	0.09837	0.99063	0.00
38:58.3	Data point 66	0.50000 mL	0.19334 mL	0.19259 mL	1.15005 mL	0.02500 mL	7.071	0.10035	0.98967	0.00
39:39.3	Data point 67	0.50000 mL	0.19334 mL	0.19273 mL	1.15005 mL	0.02500 mL	7.362	0.09739	0.97312	0.00
40:18.2	Data point 68	0.50000 mL	0.19334 mL	0.19287 mL	1.15005 mL	0.02500 mL	7.628	0.09805	0.97970	0.00
40:57.7	Data point 69	0.50000 mL	0.19334 mL	0.19301 mL	1.15005 mL	0.02500 mL	7.890	0.09989	0.98284	0.00
41:37.8	Data point 70	0.50000 mL	0.19334 mL	0.19318 mL	1.15005 mL	0.02500 mL	8.195	0.09900	0.97814	0.00
42:20.8	Data point 71	0.50000 mL	0.19334 mL	0.19334 mL	1.15005 mL	0.02500 mL	8.530	0.09664	0.98007	0.00

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SI
43:05.3	Data point 72	0.50000 mL	0.19334 mL	0.19348 mL	1.15005 mL	0.02500 mL	8.862	0.09418	0.98569	0.
43:41.7	Data point 73	0.50000 mL	0.19334 mL	0.19365 mL	1.15005 mL	0.02500 mL	9.163	0.09925	0.98365	0.
44:22.0	Data point 74	0.50000 mL	0.19334 mL	0.19384 mL	1.15005 mL	0.02500 mL	9.403	0.09820	0.96242	0.
44:57.0	Data point 75	0.50000 mL	0.19334 mL	0.19419 mL	1.15005 mL	0.02500 mL	9.614	0.09205	0.96674	0.
45:30.6	Data point 76	0.50000 mL	0.19334 mL	0.19447 mL	1.15005 mL	0.02500 mL	9.827	0.06575	0.97089	0.
45:52.3	Data point 77	0.50000 mL	0.19334 mL	0.19471 mL	1.15005 mL	0.02500 mL	10.031	0.04335	0.97625	0.
46:24.4	Data point 78	0.50000 mL	0.19334 mL	0.19506 mL	1.15005 mL	0.02500 mL	10.231	0.02376	0.93736	0.
46:56.6	Data point 79	0.50000 mL	0.19334 mL	0.19553 mL	1.15005 mL	0.02500 mL	10.429	0.01865	0.93667	0.
47:28.7	Data point 80	0.50000 mL	0.19334 mL	0.19617 mL	1.15005 mL	0.02500 mL	10.624	0.00749	0.83005	0.
47:45.4	Data point 81	0.50000 mL	0.19334 mL	0.19704 mL	1.15005 mL	0.02500 mL	10.839	0.00505	0.79553	0.
48:02.1	Data point 82	0.50000 mL	0.19334 mL	0.19847 mL	1.15005 mL	0.02500 mL	11.058	0.00179	0.27424	0.
48:18.8	Data point 83	0.50000 mL	0.19334 mL	0.20082 mL	1.15005 mL	0.02500 mL	11.246	0.00719	0.81073	0.
48:35.6	Data point 84	0.50000 mL	0.19334 mL	0.20444 mL	1.15005 mL	0.02500 mL	11.429	0.00340	0.52423	0.
48:52.3	Data point 85	0.50000 mL	0.19334 mL	0.20997 mL	1.15005 mL	0.02500 mL	11.619	0.00710	0.73496	0.
49:09.2	Data point 86	0.50000 mL	0.19334 mL	0.21860 mL	1.15005 mL	0.02500 mL	11.805	0.00367	0.39432	0.
49:26.1	Data point 87	0.50000 mL	0.19334 mL	0.23210 mL	1.15005 mL	0.02500 mL	11.988	0.00362	0.43612	0.
49:43.0	Data point 88	0.50000 mL	0.19334 mL	0.23758 mL	1.15005 mL	0.02500 mL	12.047	0.00577	0.75458	0.
51:50.1	Reference spectrum									
52:58.3	Data point 90	0.83996 mL	0.33483 mL	0.23761 mL	1.15005 mL	0.02500 mL	1.987	-0.09876	0.98599	0.
53:42.9	Data point 91	0.83996 mL	0.33483 mL	0.27587 mL	1.15005 mL	0.02500 mL	2.181	-0.00579	0.52710	0.
54:10.4	Data point 92	0.83996 mL	0.33483 mL	0.29694 mL	1.15005 mL	0.02500 mL	2.379	0.00234	0.11016	0.
54:27.4	Data point 93	0.83996 mL	0.33483 mL	0.30974 mL	1.15005 mL	0.02500 mL	2.566	-0.01701	0.86551	0.
54:44.2	Data point 94	0.83996 mL	0.33483 mL	0.31809 mL	1.15005 mL	0.02500 mL	2.748	0.00081	0.00429	0.
55:01.1	Data point 95	0.83996 mL	0.33483 mL	0.32349 mL	1.15005 mL	0.02500 mL	2.936	-0.00425	0.29064	0.
55:17.9	Data point 96	0.83996 mL	0.33483 mL	0.32700 mL	1.15005 mL	0.02500 mL	3.121	-0.01662	0.83449	0.
55:34.6	Data point 97	0.83996 mL	0.33483 mL	0.32930 mL	1.15005 mL	0.02500 mL	3.298	-0.00866	0.53756	0.
55:51.3	Data point 98	0.83996 mL	0.33483 mL	0.33081 mL	1.15005 mL	0.02500 mL	3.426	-0.00171	0.08882	0.
56:23.4	Data point 99	0.83996 mL	0.33483 mL	0.33224 mL	1.15005 mL	0.02500 mL	3.675	0.00595	0.67554	0.
56:50.3	Data point 100	0.83996 mL	0.33483 mL	0.33281 mL	1.15005 mL	0.02500 mL	3.867	0.01093	0.89224	0.
57:07.0	Data point 101	0.83996 mL	0.33483 mL	0.33321 mL	1.15005 mL	0.02500 mL	4.120	-0.00252	0.05659	0.
57:28.8	Data point 102	0.83996 mL	0.33483 mL	0.33363 mL	1.15005 mL	0.02500 mL	4.497	-0.00454	0.08769	0.
57:50.5	Data point 103	0.83996 mL	0.33483 mL	0.33384 mL	1.15005 mL	0.02500 mL	4.759	0.03419	0.95872	0.
58:12.4	Data point 104	0.83996 mL	0.33483 mL	0.33398 mL	1.15005 mL	0.02500 mL	4.967	0.08527	0.98858	0.
58:39.3	Data point 105	0.83996 mL	0.33483 mL	0.33410 mL	1.15005 mL	0.02500 mL	5.210	0.09671	0.99101	0.
59:11.6	Data point 106	0.83996 mL	0.33483 mL	0.33422 mL	1.15005 mL	0.02500 mL	5.513	0.09710	0.97457	0.
59:40.9	Data point 107	0.83996 mL	0.33483 mL	0.33431 mL	1.15005 mL	0.02500 mL	5.782	0.09877	0.98203	0.
1:00:20.8	Data point 108	0.83996 mL	0.33483 mL	0.33441 mL	1.15005 mL	0.02500 mL	6.100	0.09969	0.98809	0.
1:00:54.1	Data point 109	0.83996 mL	0.33483 mL	0.33450 mL	1.15005 mL	0.02500 mL	6.321	0.08279	0.76909	0.
1:01:15.8	Data point 110	0.83996 mL	0.33483 mL	0.33459 mL	1.15005 mL	0.02500 mL	6.548	0.07039	0.65422	0.
1:01:37.6	Data point 111	0.83996 mL	0.33483 mL	0.33471 mL	1.15005 mL	0.02500 mL	6.812	0.04591	0.28713	0.
1:02:05.0	Data point 112	0.83996 mL	0.33483 mL	0.33485 mL	1.15005 mL	0.02500 mL	7.057	0.08431	0.86462	0.
1:02:32.4	Data point 113	0.83996 mL	0.33483 mL	0.33499 mL	1.15005 mL	0.02500 mL	7.298	0.08343	0.81431	0.
1:03:06.0	Data point 114	0.83996 mL	0.33483 mL	0.33514 mL	1.15005 mL	0.02500 mL	7.535	0.08886	0.92103	0.
1:03:39.8	Data point 115	0.83996 mL	0.33483 mL	0.33528 mL	1.15005 mL	0.02500 mL	7.802	0.09817	0.95470	0.
1:04:16.3	Data point 116	0.83996 mL	0.33483 mL	0.33542 mL	1.15005 mL	0.02500 mL	8.100	0.09469	0.95852	0.
1:04:54.4	Data point 117	0.83996 mL	0.33483 mL	0.33556 mL	1.15005 mL	0.02500 mL	8.419	0.09873	0.95441	0.
1:05:33.4	Data point 118	0.83996 mL	0.33483 mL	0.33570 mL	1.15005 mL	0.02500 mL	8.710	0.09479	0.96226	0.
1:06:06.4	Data point 119	0.83996 mL	0.33483 mL	0.33584 mL	1.15005 mL	0.02500 mL	8.949	0.09165	0.93096	0.
1:06:41.5	Data point 120	0.83996 mL	0.33483 mL	0.33601 mL	1.15005 mL	0.02500 mL	9.185	0.08075	0.94036	0.
1:07:13.4	Data point 121	0.83996 mL	0.33483 mL	0.33620 mL	1.15005 mL	0.02500 mL	9.406	0.05660	0.96063	0.
1:07:35.2	Data point 122	0.83996 mL	0.33483 mL	0.33638 mL	1.15005 mL	0.02500 mL	9.601	0.02231	0.95508	0.
1:08:07.2	Data point 123	0.83996 mL	0.33483 mL	0.33666 mL	1.15005 mL	0.02500 mL	9.797	0.01732	0.87678	0.
1:08:39.3	Data point 124	0.83996 mL	0.33483 mL	0.33704 mL	1.15005 mL	0.02500 mL	9.994	0.02135	0.94744	0.
1:09:11.3	Data point 125	0.83996 mL	0.33483 mL	0.33753 mL	1.15005 mL	0.02500 mL	10.191	0.01065	0.91235	0.
1:09:43.6	Data point 126	0.83996 mL	0.33483 mL	0.33826 mL	1.15005 mL	0.02500 mL	10.384	0.00562	0.66301	0.
1:10:05.5	Data point 127	0.83996 mL	0.33483 mL	0.33946 mL	1.15005 mL	0.02500 mL	10.611	-0.01477	0.84873	0.
1:10:37.7	Data point 128	0.83996 mL	0.33483 mL	0.34099 mL	1.15005 mL	0.02500 mL	10.819	-0.00454	0.61071	0.
1:11:04.7	Data point 129	0.83996 mL	0.33483 mL	0.34271 mL	1.15005 mL	0.02500 mL	11.009	-0.00196	0.21283	0.

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:11:31.8	Data point 130	0.83996 mL	0.33483 mL	0.34591 mL	1.15005 mL	0.02500 mL	11.201	-0.00222	0.22145	0.0002
1:11:48.6	Data point 131	0.83996 mL	0.33483 mL	0.35089 mL	1.15005 mL	0.02500 mL	11.390	-0.01446	0.84982	0.0007
1:12:05.6	Data point 132	0.83996 mL	0.33483 mL	0.35866 mL	1.15005 mL	0.02500 mL	11.579	-0.01315	0.83717	0.0007
1:12:22.7	Data point 133	0.83996 mL	0.33483 mL	0.37081 mL	1.15005 mL	0.02500 mL	11.777	-0.00757	0.43491	0.0005
1:12:39.8	Data point 134	0.83996 mL	0.33483 mL	0.39031 mL	1.15005 mL	0.02500 mL	11.969	-0.01415	0.71005	0.0008
1:12:56.8	Data point 135	0.83996 mL	0.33483 mL	0.40122 mL	1.15005 mL	0.02500 mL	12.046	-0.00446	0.44815	0.0003
1:15:02.2	Assay volumes	1.08996 mL	0.50520 mL	0.40122 mL	1.15005 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.144	5/22/2018 12:19:28 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus S	0.9948	5/22/2018 12:19:28 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jH	1.0	5/22/2018 12:19:28 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jOH	-0.8	5/22/2018 12:19:28 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Base concentration factor	1.012	5/22/2018 12:19:28 PM	C:\Sirius_T3\KOH18D10.t3r
Acid concentration factor	0.998	5/22/2018 12:19:28 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	5/15/2018 2:12:22 PM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	3-22-18	5/15/2018 2:12:48 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Titrant	Base (0.5 M KOH)	3-22-18	5/15/2018 2:12:34 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	2-8-18	5/15/2018 2:14:14 PM
Port B	Cyclohexane		4/10/2018 8:40:51 AM
Port C	MeCN (50%, 0.15 M KCl)	4-16-18	5/15/2018 2:14:20 PM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	5/15/2018 2:12:54 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	1-31-2018	4/9/2018 9:14:11 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-10.62 mV		5/22/2018 12:19:52 PM
Filling solution	3M KCl	KCL095	5/21/2018 8:57:01 AM
Liquids			
Wash 1	50% IPA:50% Water		5/22/2018 8:38:15 AM
Wash 2	0.5% Trition X-100 in H20		5/22/2018 8:38:18 AM
Buffer position 1	pH7 Wash		5/22/2018 8:38:22 AM
Buffer position 2	pH 7		5/22/2018 8:38:25 AM
Storage position			5/22/2018 8:38:32 AM
Wash water	3.5e+003 mL	5-15-18	5/15/2018 2:11:48 PM
Waste	7e+003 mL		3/19/2018 10:48:12 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	897:26:49		11/23/2010 12:22:28 PM
Calibrated on	5/21/2018 2:44:22 PM		
Integration time	19		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location B1

UV-metric psKa_0417936-0002 Titration 1 of 3 18E-22012 Points 4 to 43

Results

pKa 1	**4.76**
pKa 2	**9.10**
RMSD	**0.036 0.029 0.023**
Chi squared	**0.1560**
PCA calculated number of pKas	**4**
Average ionic strength	**0.158 M**
Average temperature	**25.0°C**
Analyte concentration range	**60.6 µM to 56.8 µM**
Methanol weight %	**49.0 %**
Dielectric constant	**56.8**
Water concentration	**25.0 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.460 to 12.540**

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

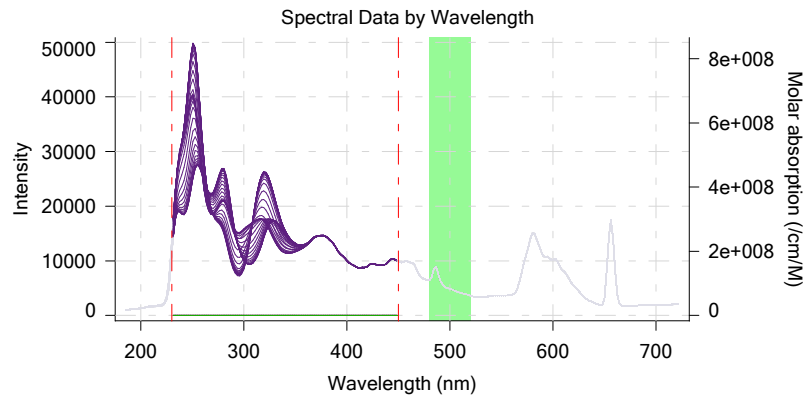
Warnings and errors

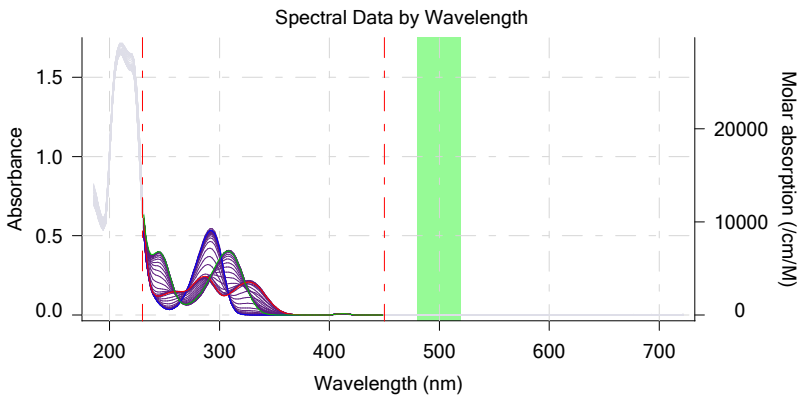
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

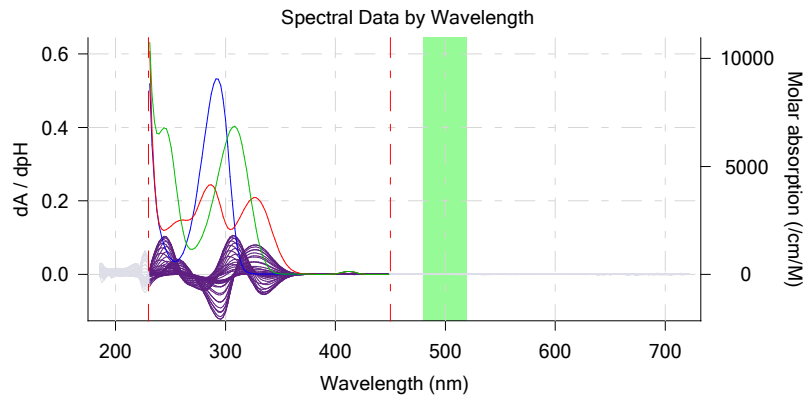
Assay Settings

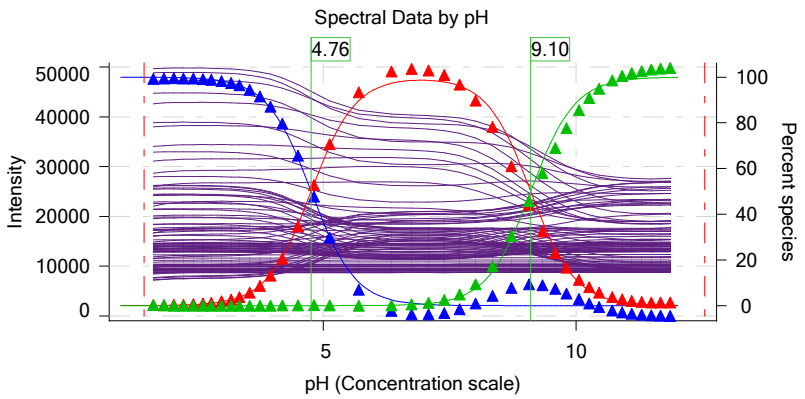
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

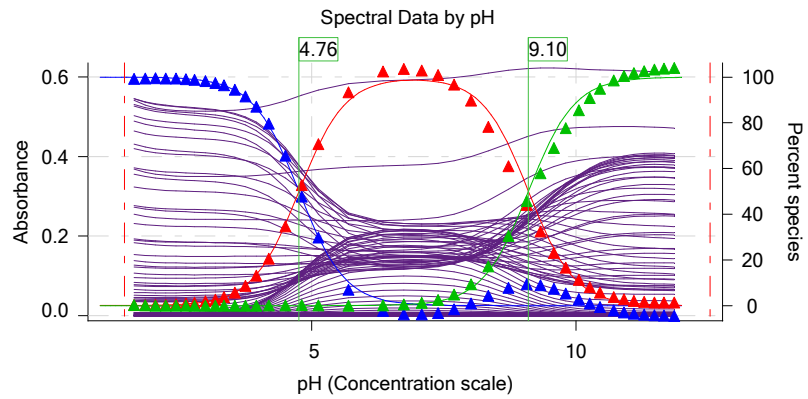
Graphs

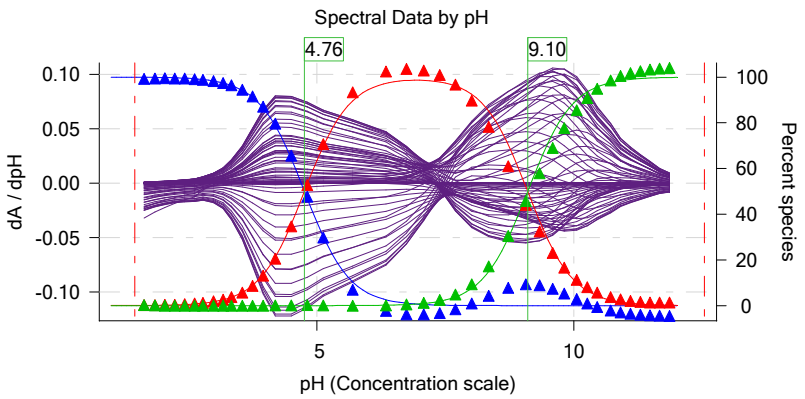






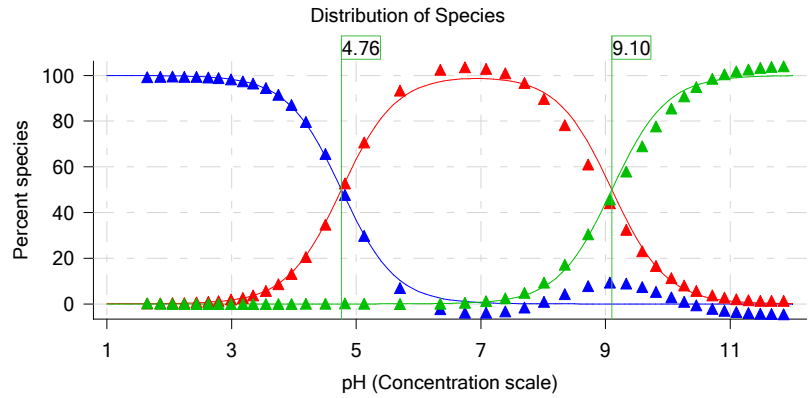


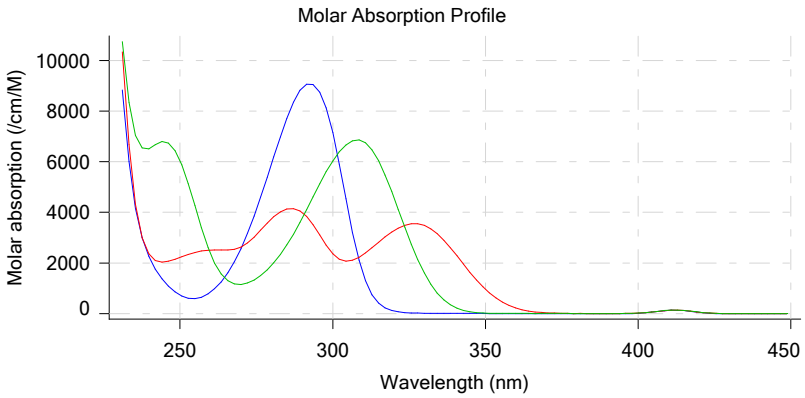


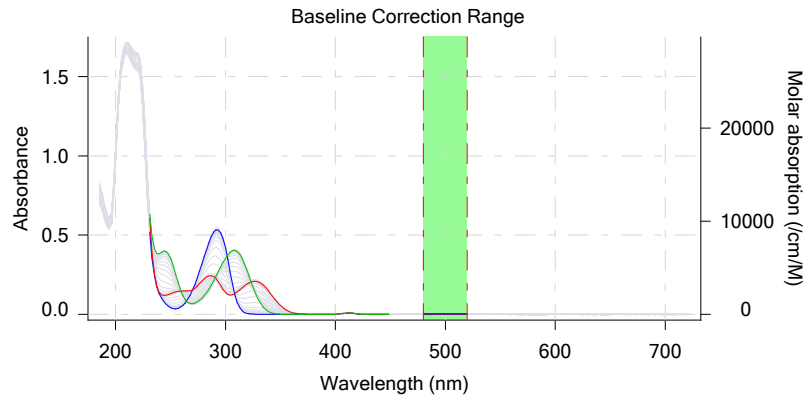


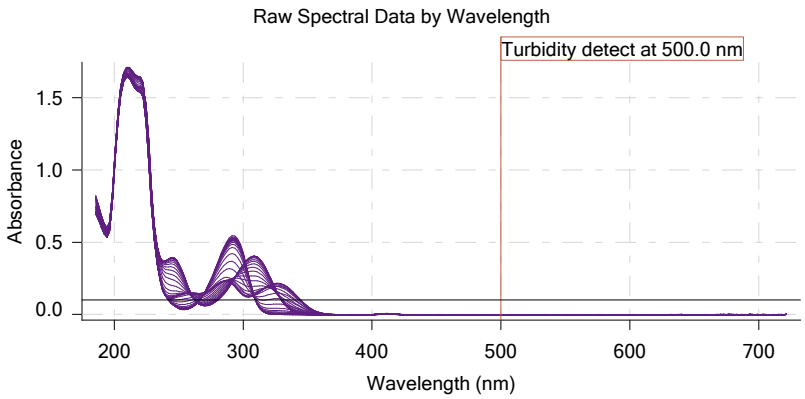
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Graphs (continued)









UV-metric psKa_0417936-0002 Titration 2 of 3 18E-22012 Points 45 to 88

Results

pKa 1	**4.78**
pKa 2	**9.01**
RMSD	**0.045 0.033 0.031**
Chi squared	**0.2304**
PCA calculated number of pKas	**3**
Average ionic strength	**0.168 M**
Average temperature	**25.0°C**
Analyte concentration range	**49.2 µM to 46.2 µM**
Methanol weight %	**38.9 %**
Dielectric constant	**61.5**
Water concentration	**30.6 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.474 to 12.543**

Warnings and errors

Errors None
Warnings PCA calculation disagrees with predicted number of pKas

Assay Settings

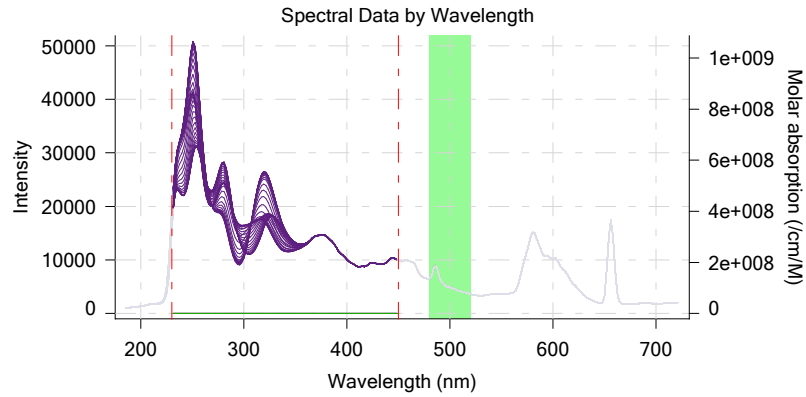
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				

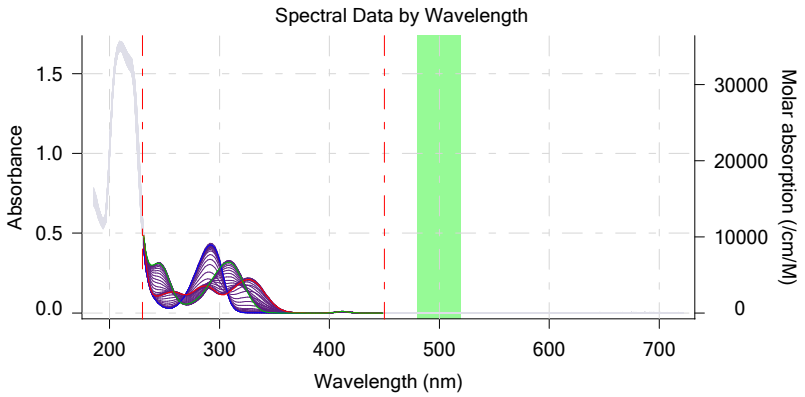
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

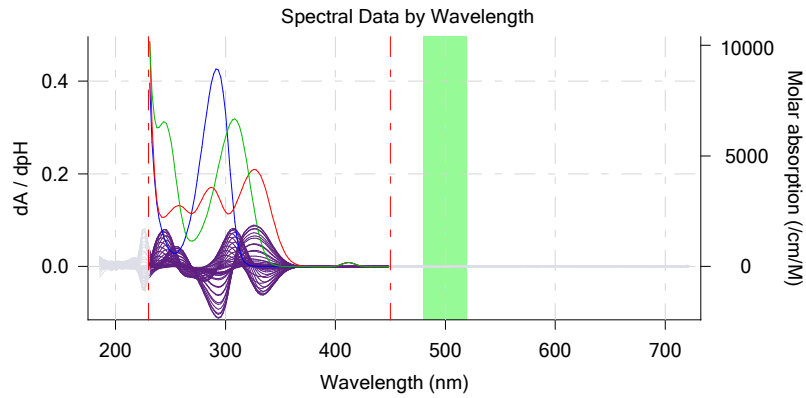
Assay Settings (continued)

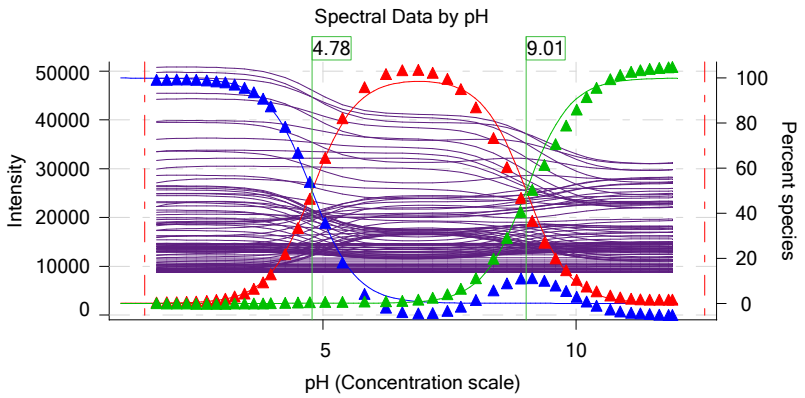
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

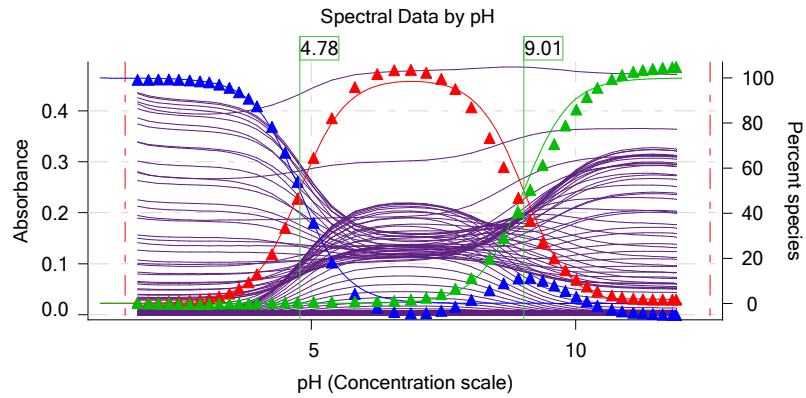
Graphs

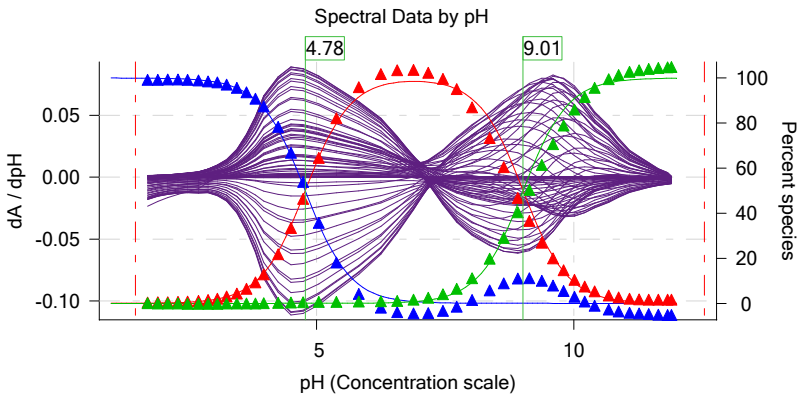






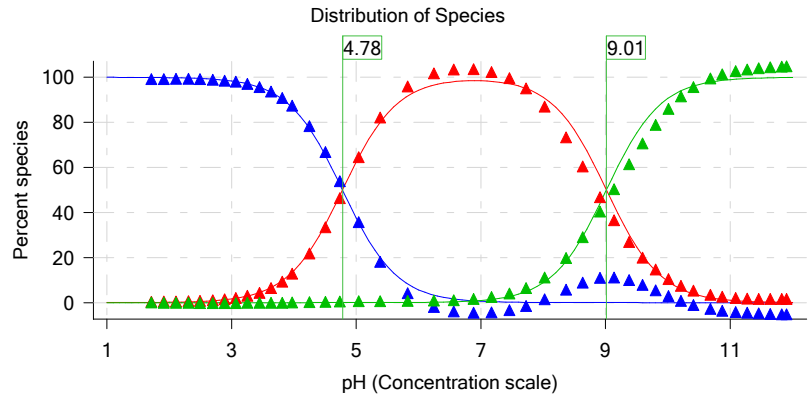


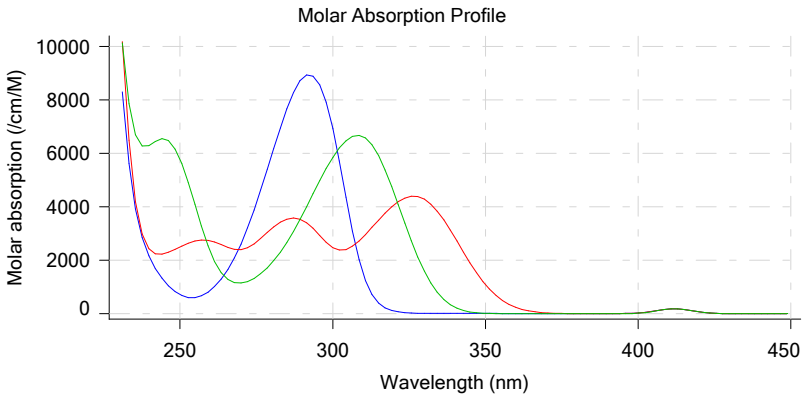


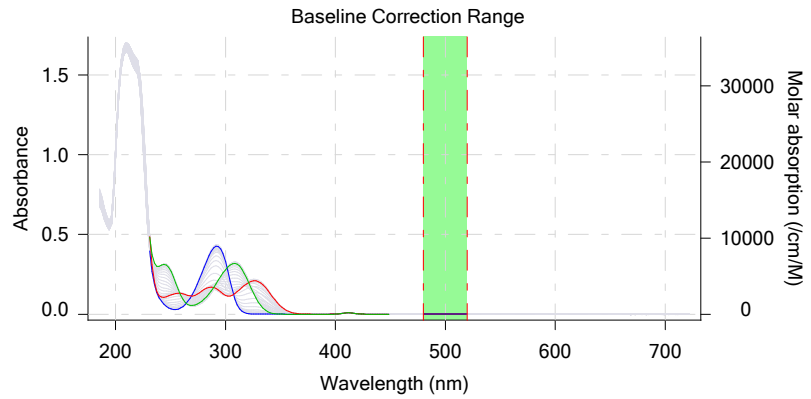


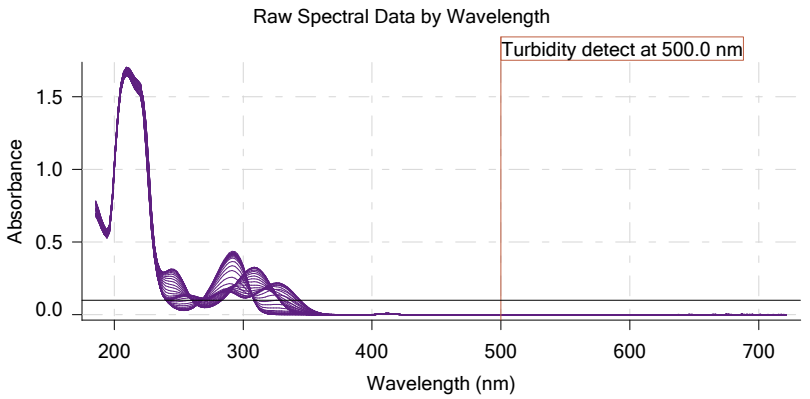
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Graphs (continued)









UV-metric psKa_0417936-0002 Titration 3 of 3 18E-22012 Points 90 to 134

Results

pKa 1	**4.82**
pKa 2	**8.96**
RMSD	**0.045 0.031 0.035**
Chi squared	**0.2714**
PCA calculated number of pKas	**3**
Average ionic strength	**0.174 M**
Average temperature	**25.0°C**
Analyte concentration range	**37.6 µM to 35.6 µM**
Methanol weight %	**29.3 %**
Dielectric constant	**65.8**
Water concentration	**36.3 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.531 to 12.523**

Warnings and errors

Errors None
Warnings PCA calculation disagrees with predicted number of pKas

Assay Settings

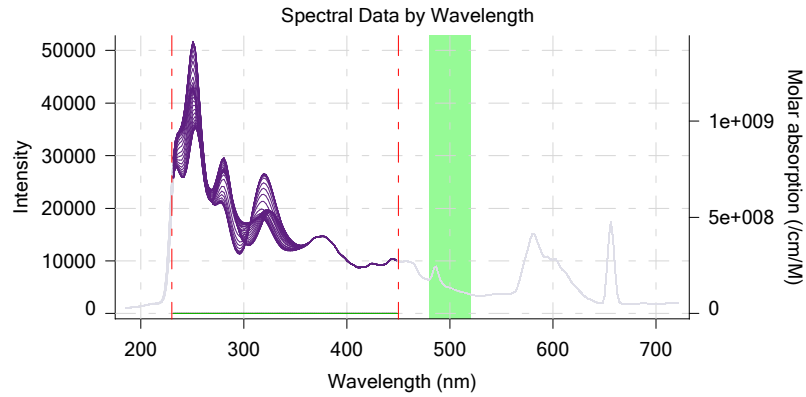
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				

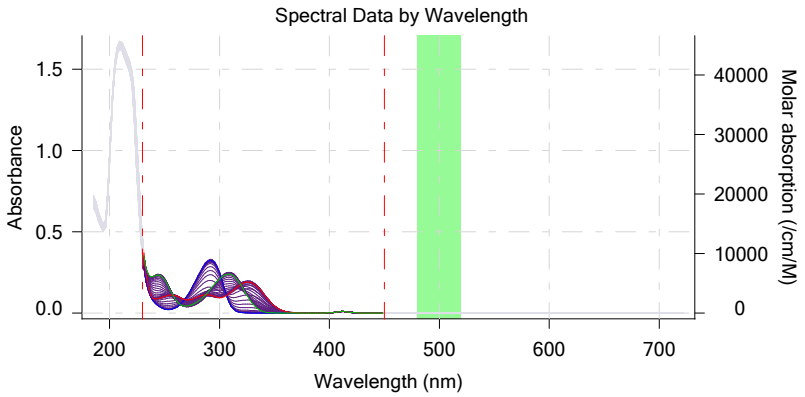
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

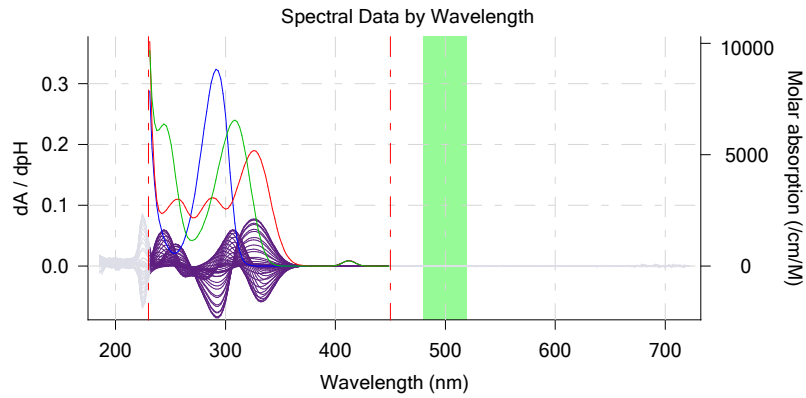
Assay Settings (continued)

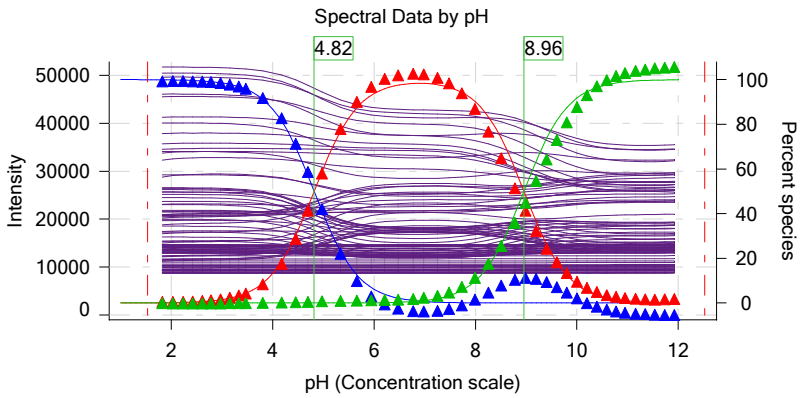
Setting	Value	Original Value	Date/Time changed	Imported from
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

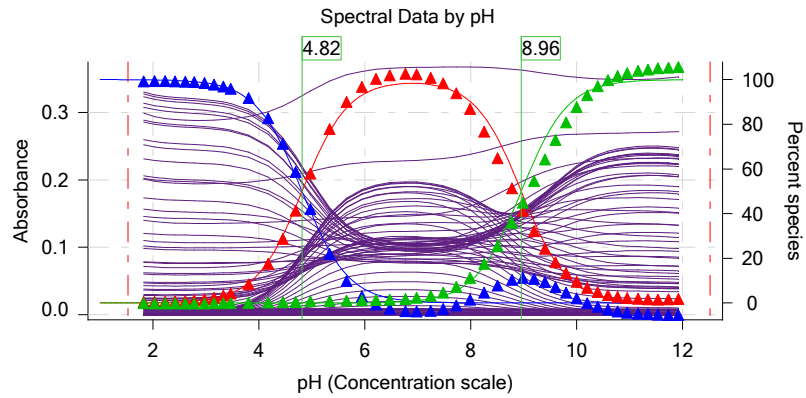
Graphs

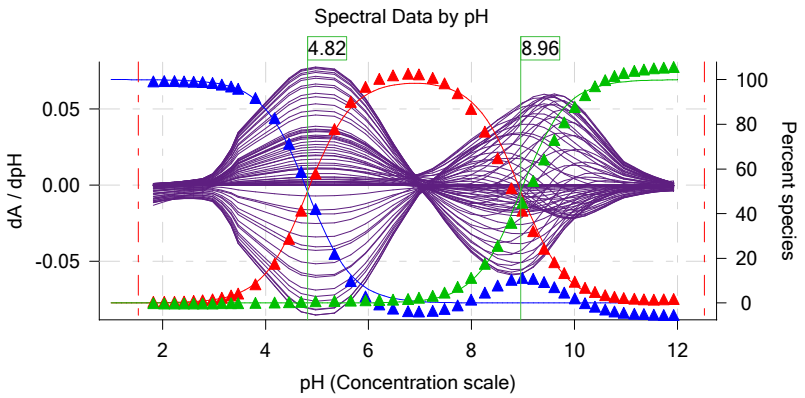






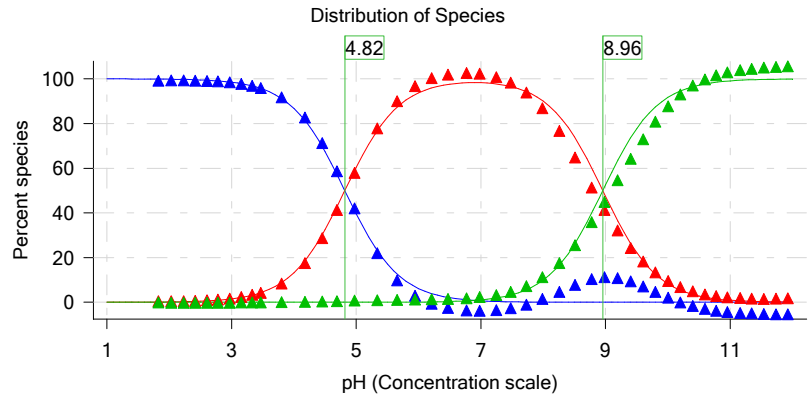


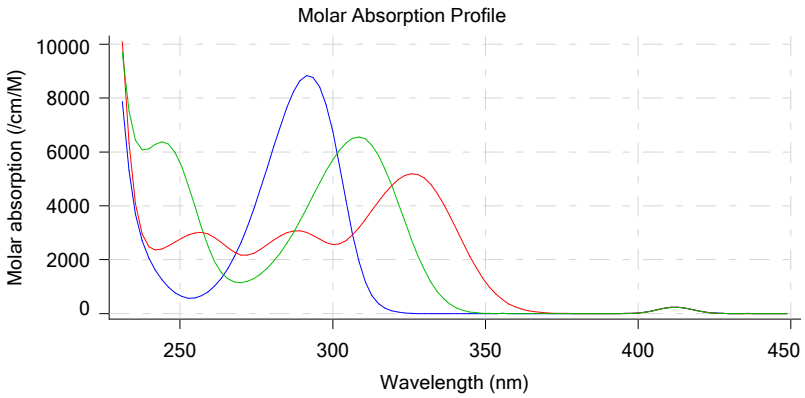


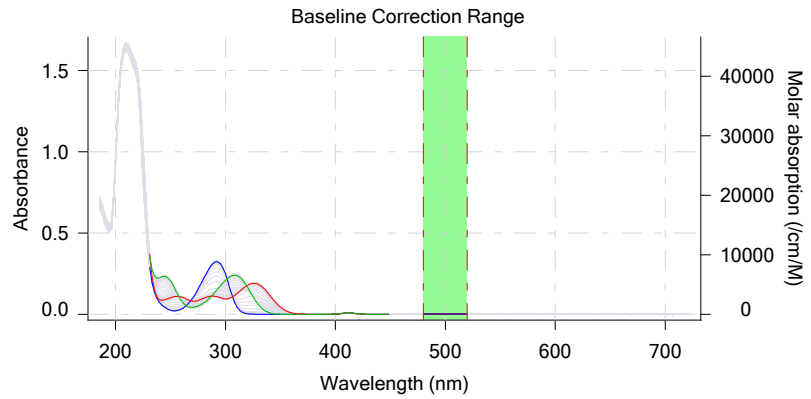


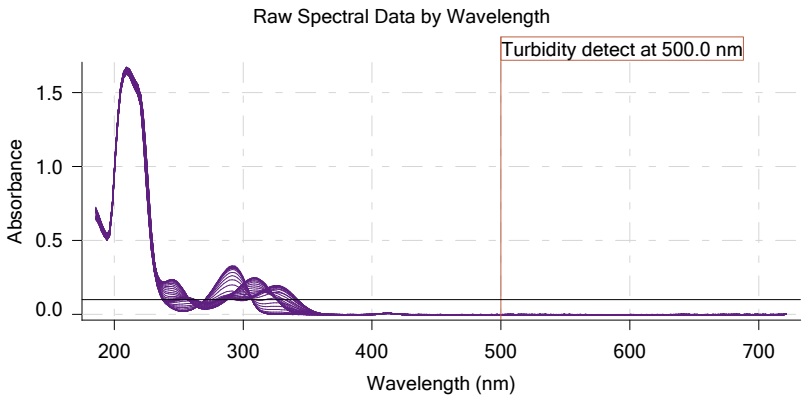
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Graphs (continued)









UV-metric psKa_0417936-0002 18E-22012 Assay 2 of 3

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	Pyridoxine HCl	5/22/2018 9:07:27 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	5/22/2018 9:07:27 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.048630 M	5/22/2018 9:07:27 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	205.64	5/22/2018 9:07:35 AM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	5/22/2018 9:07:27 AM	User entered value
Sample is a	Ampholyte	5/22/2018 9:07:27 AM	User entered value
pKa 1	4.90	5/22/2018 9:07:27 AM	User entered value
Type	Base	5/22/2018 9:07:27 AM	User entered value
pKa 2	8.80	5/22/2018 9:07:27 AM	User entered value
Type	Acid	5/22/2018 9:07:27 AM	User entered value
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	5/22/2018 9:07:27 AM	User entered value
logP (X -)	-10.00		Default value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squar
3:46.9	Dark spectrum								
3:48.3	Reference spectrum								
4:15.9	Volume reset due to vial change								
5:00.2	Initial pH = 7.86								
6:10.8	Data point 4	0.34995 mL	0.07681 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.960	-0.00262	0.18608
6:39.7	Data point 5	0.34995 mL	0.07681 mL	0.02785 mL	1.15005 mL	0.02500 mL	2.161	0.00506	0.48029
6:56.7	Data point 6	0.34995 mL	0.07681 mL	0.04461 mL	1.15005 mL	0.02500 mL	2.352	0.02921	0.81795
7:13.7	Data point 7	0.34995 mL	0.07681 mL	0.05536 mL	1.15005 mL	0.02500 mL	2.541	0.00204	0.06226
7:30.5	Data point 8	0.34995 mL	0.07681 mL	0.06232 mL	1.15005 mL	0.02500 mL	2.731	0.02084	0.95103
7:47.2	Data point 9	0.34995 mL	0.07681 mL	0.06677 mL	1.15005 mL	0.02500 mL	2.918	0.02803	0.94078
8:04.0	Data point 10	0.34995 mL	0.07681 mL	0.06964 mL	1.15005 mL	0.02500 mL	3.080	0.01520	0.93331
8:36.1	Data point 11	0.34995 mL	0.07681 mL	0.07154 mL	1.15005 mL	0.02500 mL	3.279	0.01557	0.93093
8:52.9	Data point 12	0.34995 mL	0.07681 mL	0.07279 mL	1.15005 mL	0.02500 mL	3.465	0.00821	0.58554
9:09.5	Data point 13	0.34995 mL	0.07681 mL	0.07361 mL	1.15005 mL	0.02500 mL	3.628	0.01544	0.87596
9:41.6	Data point 14	0.34995 mL	0.07681 mL	0.07439 mL	1.15005 mL	0.02500 mL	3.832	0.03961	0.98583
10:13.7	Data point 15	0.34995 mL	0.07681 mL	0.07484 mL	1.15005 mL	0.02500 mL	4.032	0.05603	0.99076
10:35.5	Data point 16	0.34995 mL	0.07681 mL	0.07512 mL	1.15005 mL	0.02500 mL	4.235	0.08548	0.97529
10:57.3	Data point 17	0.34995 mL	0.07681 mL	0.07538 mL	1.15005 mL	0.02500 mL	4.468	0.10052	0.99340
11:31.3	Data point 18	0.34995 mL	0.07681 mL	0.07561 mL	1.15005 mL	0.02500 mL	4.775	0.10035	0.99387
12:17.3	Data point 19	0.34995 mL	0.07681 mL	0.07578 mL	1.15005 mL	0.02500 mL	5.084	0.09837	0.98761
13:10.9	Data point 20	0.34995 mL	0.07681 mL	0.07599 mL	1.15005 mL	0.02500 mL	5.391	0.09080	0.92070
14:02.8	Data point 21	0.34995 mL	0.07681 mL	0.07622 mL	1.15005 mL	0.02500 mL	5.958	0.10038	0.99058
15:10.7	Data point 22	0.34995 mL	0.07681 mL	0.07636 mL	1.15005 mL	0.02500 mL	6.599	0.10100	0.99618
16:12.1	Data point 23	0.34995 mL	0.07681 mL	0.07651 mL	1.15005 mL	0.02500 mL	6.992	0.10062	0.98872
17:04.0	Data point 24	0.34995 mL	0.07681 mL	0.07665 mL	1.15005 mL	0.02500 mL	7.325	0.10067	0.99449
17:54.0	Data point 25	0.34995 mL	0.07681 mL	0.07679 mL	1.15005 mL	0.02500 mL	7.629	0.09907	0.98294
18:39.9	Data point 26	0.34995 mL	0.07681 mL	0.07695 mL	1.15005 mL	0.02500 mL	7.933	0.09862	0.98671
19:26.5	Data point 27	0.34995 mL	0.07681 mL	0.07712 mL	1.15005 mL	0.02500 mL	8.245	0.09931	0.98811
20:13.1	Data point 28	0.34995 mL	0.07681 mL	0.07726 mL	1.15005 mL	0.02500 mL	8.573	0.09687	0.98688
20:59.8	Data point 29	0.34995 mL	0.07681 mL	0.07740 mL	1.15005 mL	0.02500 mL	8.945	0.09799	0.98364
21:42.8	Data point 30	0.34995 mL	0.07681 mL	0.07754 mL	1.15005 mL	0.02500 mL	9.288	0.09809	0.97889
22:23.3	Data point 31	0.34995 mL	0.07681 mL	0.07766 mL	1.15005 mL	0.02500 mL	9.549	0.09709	0.97913
23:01.1	Data point 32	0.34995 mL	0.07681 mL	0.07780 mL	1.15005 mL	0.02500 mL	9.800	0.09788	0.97909
23:34.0	Data point 33	0.34995 mL	0.07681 mL	0.07796 mL	1.15005 mL	0.02500 mL	10.021	0.09974	0.97306
23:56.3	Data point 34	0.34995 mL	0.07681 mL	0.07817 mL	1.15005 mL	0.02500 mL	10.263	0.05574	0.96090
24:28.3	Data point 35	0.34995 mL	0.07681 mL	0.07850 mL	1.15005 mL	0.02500 mL	10.466	0.03725	0.96369
24:55.2	Data point 36	0.34995 mL	0.07681 mL	0.07893 mL	1.15005 mL	0.02500 mL	10.659	0.01482	0.94120
25:11.9	Data point 37	0.34995 mL	0.07681 mL	0.07959 mL	1.15005 mL	0.02500 mL	10.915	0.01430	0.91822
25:38.8	Data point 38	0.34995 mL	0.07681 mL	0.08076 mL	1.15005 mL	0.02500 mL	11.107	0.00457	0.50168
25:55.6	Data point 39	0.34995 mL	0.07681 mL	0.08262 mL	1.15005 mL	0.02500 mL	11.295	0.00375	0.77087
26:12.3	Data point 40	0.34995 mL	0.07681 mL	0.08549 mL	1.15005 mL	0.02500 mL	11.485	0.00291	0.24561
26:29.1	Data point 41	0.34995 mL	0.07681 mL	0.08996 mL	1.15005 mL	0.02500 mL	11.673	-0.00043	0.01418
26:45.9	Data point 42	0.34995 mL	0.07681 mL	0.09692 mL	1.15005 mL	0.02500 mL	11.852	-0.00055	0.01631
27:02.9	Data point 43	0.34995 mL	0.07681 mL	0.10750 mL	1.15005 mL	0.02500 mL	12.040	0.00529	0.56810
28:45.1	Reference spectrum								
29:49.6	Data point 45	0.50000 mL	0.19196 mL	0.10753 mL	1.15005 mL	0.02500 mL	1.974	-0.09833	0.97177
30:19.3	Data point 46	0.50000 mL	0.19196 mL	0.13984 mL	1.15005 mL	0.02500 mL	2.170	0.00325	0.36132
30:36.4	Data point 47	0.50000 mL	0.19196 mL	0.15790 mL	1.15005 mL	0.02500 mL	2.357	0.00633	0.36424
30:53.3	Data point 48	0.50000 mL	0.19196 mL	0.16952 mL	1.15005 mL	0.02500 mL	2.553	0.00298	0.11344
31:10.2	Data point 49	0.50000 mL	0.19196 mL	0.17691 mL	1.15005 mL	0.02500 mL	2.735	-0.00019	0.00047
31:27.0	Data point 50	0.50000 mL	0.19196 mL	0.18180 mL	1.15005 mL	0.02500 mL	2.941	0.00556	0.23229
31:43.8	Data point 51	0.50000 mL	0.19196 mL	0.18478 mL	1.15005 mL	0.02500 mL	3.127	0.01379	0.85718
32:00.5	Data point 52	0.50000 mL	0.19196 mL	0.18674 mL	1.15005 mL	0.02500 mL	3.306	0.00871	0.81949
32:17.3	Data point 53	0.50000 mL	0.19196 mL	0.18801 mL	1.15005 mL	0.02500 mL	3.487	0.01813	0.94453
32:34.1	Data point 54	0.50000 mL	0.19196 mL	0.18885 mL	1.15005 mL	0.02500 mL	3.680	0.03011	0.98819
32:50.8	Data point 55	0.50000 mL	0.19196 mL	0.18939 mL	1.15005 mL	0.02500 mL	3.863	0.03366	0.93520
33:07.5	Data point 56	0.50000 mL	0.19196 mL	0.18975 mL	1.15005 mL	0.02500 mL	4.041	0.05179	0.99213
33:24.2	Data point 57	0.50000 mL	0.19196 mL	0.18998 mL	1.15005 mL	0.02500 mL	4.196	0.05519	0.99390

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SE
33:46.0	Data point 58	0.50000 mL	0.19196 mL	0.19024 mL	1.15005 mL	0.02500 mL	4.476	0.09086	0.99504	0.
34:07.8	Data point 59	0.50000 mL	0.19196 mL	0.19040 mL	1.15005 mL	0.02500 mL	4.725	0.10032	0.98974	0.
34:34.5	Data point 60	0.50000 mL	0.19196 mL	0.19052 mL	1.15005 mL	0.02500 mL	4.958	0.09910	0.96735	0.
35:11.4	Data point 61	0.50000 mL	0.19196 mL	0.19064 mL	1.15005 mL	0.02500 mL	5.257	0.09878	0.99018	0.
35:51.9	Data point 62	0.50000 mL	0.19196 mL	0.19073 mL	1.15005 mL	0.02500 mL	5.597	0.09974	0.99368	0.
36:39.3	Data point 63	0.50000 mL	0.19196 mL	0.19083 mL	1.15005 mL	0.02500 mL	6.032	0.09907	0.99027	0.
37:30.1	Data point 64	0.50000 mL	0.19196 mL	0.19092 mL	1.15005 mL	0.02500 mL	6.451	0.10056	0.99188	0.
38:18.3	Data point 65	0.50000 mL	0.19196 mL	0.19102 mL	1.15005 mL	0.02500 mL	6.765	0.09938	0.99220	0.
39:02.7	Data point 66	0.50000 mL	0.19196 mL	0.19113 mL	1.15005 mL	0.02500 mL	7.082	0.09974	0.99271	0.
39:45.2	Data point 67	0.50000 mL	0.19196 mL	0.19128 mL	1.15005 mL	0.02500 mL	7.365	0.09701	0.97636	0.
40:23.6	Data point 68	0.50000 mL	0.19196 mL	0.19142 mL	1.15005 mL	0.02500 mL	7.651	0.09806	0.98564	0.
41:02.0	Data point 69	0.50000 mL	0.19196 mL	0.19156 mL	1.15005 mL	0.02500 mL	7.913	0.09750	0.98159	0.
41:41.6	Data point 70	0.50000 mL	0.19196 mL	0.19170 mL	1.15005 mL	0.02500 mL	8.209	0.09558	0.97711	0.
42:25.2	Data point 71	0.50000 mL	0.19196 mL	0.19184 mL	1.15005 mL	0.02500 mL	8.551	0.09943	0.98562	0.
43:04.2	Data point 72	0.50000 mL	0.19196 mL	0.19196 mL	1.15005 mL	0.02500 mL	8.817	0.09656	0.96151	0.
43:40.7	Data point 73	0.50000 mL	0.19196 mL	0.19207 mL	1.15005 mL	0.02500 mL	9.090	0.09529	0.96154	0.
44:15.0	Data point 74	0.50000 mL	0.19196 mL	0.19219 mL	1.15005 mL	0.02500 mL	9.312	0.09918	0.97807	0.
44:45.3	Data point 75	0.50000 mL	0.19196 mL	0.19236 mL	1.15005 mL	0.02500 mL	9.551	0.09905	0.96394	0.
45:18.0	Data point 76	0.50000 mL	0.19196 mL	0.19254 mL	1.15005 mL	0.02500 mL	9.767	0.06335	0.96837	0.
45:50.0	Data point 77	0.50000 mL	0.19196 mL	0.19278 mL	1.15005 mL	0.02500 mL	9.972	0.04059	0.95054	0.
46:11.9	Data point 78	0.50000 mL	0.19196 mL	0.19306 mL	1.15005 mL	0.02500 mL	10.179	0.02531	0.97189	0.
46:44.0	Data point 79	0.50000 mL	0.19196 mL	0.19356 mL	1.15005 mL	0.02500 mL	10.377	0.01925	0.96277	0.
47:15.8	Data point 80	0.50000 mL	0.19196 mL	0.19424 mL	1.15005 mL	0.02500 mL	10.571	0.00903	0.45590	0.
47:42.8	Data point 81	0.50000 mL	0.19196 mL	0.19574 mL	1.15005 mL	0.02500 mL	10.841	0.00473	0.70575	0.
48:09.8	Data point 82	0.50000 mL	0.19196 mL	0.19725 mL	1.15005 mL	0.02500 mL	11.033	0.00100	0.06278	0.
48:26.6	Data point 83	0.50000 mL	0.19196 mL	0.19946 mL	1.15005 mL	0.02500 mL	11.242	0.00200	0.18278	0.
48:43.4	Data point 84	0.50000 mL	0.19196 mL	0.20303 mL	1.15005 mL	0.02500 mL	11.424	-0.00038	0.01035	0.
49:00.2	Data point 85	0.50000 mL	0.19196 mL	0.20849 mL	1.15005 mL	0.02500 mL	11.607	0.00144	0.09200	0.
49:17.1	Data point 86	0.50000 mL	0.19196 mL	0.21689 mL	1.15005 mL	0.02500 mL	11.789	0.00342	0.43917	0.
49:34.1	Data point 87	0.50000 mL	0.19196 mL	0.22987 mL	1.15005 mL	0.02500 mL	11.971	0.00755	0.66120	0.
49:50.9	Data point 88	0.50000 mL	0.19196 mL	0.23676 mL	1.15005 mL	0.02500 mL	12.043	-0.00055	0.01556	0.
51:52.8	Reference spectrum									
53:01.0	Data point 90	0.83996 mL	0.33069 mL	0.23678 mL	1.15005 mL	0.02500 mL	2.031	-0.08808	0.98668	0.
53:44.6	Data point 91	0.83996 mL	0.33069 mL	0.27119 mL	1.15005 mL	0.02500 mL	2.232	-0.00563	0.62691	0.
54:12.1	Data point 92	0.83996 mL	0.33069 mL	0.28975 mL	1.15005 mL	0.02500 mL	2.426	0.00057	0.00484	0.
54:29.1	Data point 93	0.83996 mL	0.33069 mL	0.30115 mL	1.15005 mL	0.02500 mL	2.611	-0.02655	0.89412	0.
54:45.9	Data point 94	0.83996 mL	0.33069 mL	0.30870 mL	1.15005 mL	0.02500 mL	2.798	-0.03851	0.77316	0.
55:02.7	Data point 95	0.83996 mL	0.33069 mL	0.31355 mL	1.15005 mL	0.02500 mL	2.966	-0.00076	0.00639	0.
55:29.8	Data point 96	0.83996 mL	0.33069 mL	0.31658 mL	1.15005 mL	0.02500 mL	3.156	0.00379	0.41519	0.
55:46.6	Data point 97	0.83996 mL	0.33069 mL	0.31867 mL	1.15005 mL	0.02500 mL	3.338	-0.00894	0.44445	0.
56:03.2	Data point 98	0.83996 mL	0.33069 mL	0.32004 mL	1.15005 mL	0.02500 mL	3.512	-0.00224	0.04418	0.
56:19.9	Data point 99	0.83996 mL	0.33069 mL	0.32095 mL	1.15005 mL	0.02500 mL	3.648	-0.00170	0.04527	0.
56:41.7	Data point 100	0.83996 mL	0.33069 mL	0.32220 mL	1.15005 mL	0.02500 mL	3.982	-0.02166	0.55788	0.
57:03.5	Data point 101	0.83996 mL	0.33069 mL	0.32279 mL	1.15005 mL	0.02500 mL	4.350	-0.01439	0.31696	0.
57:25.3	Data point 102	0.83996 mL	0.33069 mL	0.32307 mL	1.15005 mL	0.02500 mL	4.627	0.05170	0.84742	0.
57:52.1	Data point 103	0.83996 mL	0.33069 mL	0.32326 mL	1.15005 mL	0.02500 mL	4.862	0.09807	0.98201	0.
58:16.4	Data point 104	0.83996 mL	0.33069 mL	0.32338 mL	1.15005 mL	0.02500 mL	5.139	0.10044	0.98603	0.
58:45.1	Data point 105	0.83996 mL	0.33069 mL	0.32347 mL	1.15005 mL	0.02500 mL	5.502	0.09952	0.99014	0.
59:19.5	Data point 106	0.83996 mL	0.33069 mL	0.32356 mL	1.15005 mL	0.02500 mL	5.819	0.09839	0.98916	0.
59:51.8	Data point 107	0.83996 mL	0.33069 mL	0.32366 mL	1.15005 mL	0.02500 mL	6.103	0.08461	0.95372	0.
1:00:18.6	Data point 108	0.83996 mL	0.33069 mL	0.32375 mL	1.15005 mL	0.02500 mL	6.366	0.10097	0.99631	0.
1:00:44.9	Data point 109	0.83996 mL	0.33069 mL	0.32385 mL	1.15005 mL	0.02500 mL	6.627	0.05492	0.47103	0.
1:01:07.1	Data point 110	0.83996 mL	0.33069 mL	0.32394 mL	1.15005 mL	0.02500 mL	6.921	0.01022	0.01630	0.
1:01:29.4	Data point 111	0.83996 mL	0.33069 mL	0.32404 mL	1.15005 mL	0.02500 mL	7.131	0.05833	0.48152	0.
1:02:01.4	Data point 112	0.83996 mL	0.33069 mL	0.32418 mL	1.15005 mL	0.02500 mL	7.395	0.08476	0.89782	0.
1:02:34.0	Data point 113	0.83996 mL	0.33069 mL	0.32429 mL	1.15005 mL	0.02500 mL	7.625	0.09737	0.97849	0.
1:03:10.1	Data point 114	0.83996 mL	0.33069 mL	0.32441 mL	1.15005 mL	0.02500 mL	7.873	0.09424	0.97098	0.
1:03:42.9	Data point 115	0.83996 mL	0.33069 mL	0.32451 mL	1.15005 mL	0.02500 mL	8.130	0.09645	0.97593	0.

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
1:04:18.3	Data point 116	0.83996 mL	0.33069 mL	0.32460 mL	1.15005 mL	0.02500 mL	8.395	0.09492	0.96995	0.0047
1:04:53.8	Data point 117	0.83996 mL	0.33069 mL	0.32469 mL	1.15005 mL	0.02500 mL	8.646	0.09985	0.98247	0.0049
1:05:26.6	Data point 118	0.83996 mL	0.33069 mL	0.32481 mL	1.15005 mL	0.02500 mL	8.911	0.09333	0.97592	0.0046
1:05:57.7	Data point 119	0.83996 mL	0.33069 mL	0.32493 mL	1.15005 mL	0.02500 mL	9.117	0.09309	0.94545	0.0047
1:06:26.2	Data point 120	0.83996 mL	0.33069 mL	0.32507 mL	1.15005 mL	0.02500 mL	9.326	0.05680	0.95349	0.0028
1:06:58.2	Data point 121	0.83996 mL	0.33069 mL	0.32526 mL	1.15005 mL	0.02500 mL	9.534	0.03945	0.95262	0.0020
1:07:30.2	Data point 122	0.83996 mL	0.33069 mL	0.32549 mL	1.15005 mL	0.02500 mL	9.731	0.02642	0.90136	0.0013
1:08:02.3	Data point 123	0.83996 mL	0.33069 mL	0.32580 mL	1.15005 mL	0.02500 mL	9.925	0.01362	0.89676	0.0007
1:08:34.4	Data point 124	0.83996 mL	0.33069 mL	0.32622 mL	1.15005 mL	0.02500 mL	10.126	0.00814	0.78502	0.0004
1:09:06.4	Data point 125	0.83996 mL	0.33069 mL	0.32679 mL	1.15005 mL	0.02500 mL	10.323	0.00010	0.00079	0.0001
1:09:38.6	Data point 126	0.83996 mL	0.33069 mL	0.32759 mL	1.15005 mL	0.02500 mL	10.517	-0.00127	0.08704	0.0002
1:10:10.7	Data point 127	0.83996 mL	0.33069 mL	0.32874 mL	1.15005 mL	0.02500 mL	10.711	0.00091	0.07225	0.0001
1:10:27.4	Data point 128	0.83996 mL	0.33069 mL	0.33036 mL	1.15005 mL	0.02500 mL	10.893	-0.01567	0.87536	0.0008
1:10:44.2	Data point 129	0.83996 mL	0.33069 mL	0.33281 mL	1.15005 mL	0.02500 mL	11.068	-0.01611	0.91877	0.0008
1:11:01.0	Data point 130	0.83996 mL	0.33069 mL	0.33645 mL	1.15005 mL	0.02500 mL	11.272	-0.01619	0.83924	0.0008
1:11:17.8	Data point 131	0.83996 mL	0.33069 mL	0.34229 mL	1.15005 mL	0.02500 mL	11.456	-0.01685	0.83927	0.0009
1:11:34.6	Data point 132	0.83996 mL	0.33069 mL	0.35129 mL	1.15005 mL	0.02500 mL	11.645	-0.00973	0.51831	0.0006
1:11:51.7	Data point 133	0.83996 mL	0.33069 mL	0.36536 mL	1.15005 mL	0.02500 mL	11.836	-0.01126	0.81764	0.0006
1:12:08.9	Data point 134	0.83996 mL	0.33069 mL	0.38768 mL	1.15005 mL	0.02500 mL	12.023	-0.01291	0.77056	0.0007
1:14:14.2	Assay volumes	1.08996 mL	0.49567 mL	0.38768 mL	1.15005 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Sample Sonication				
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.144	5/22/2018 1:35:32 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus S	0.9948	5/22/2018 1:35:32 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jH	1.0	5/22/2018 1:35:32 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jOH	-0.8	5/22/2018 1:35:32 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Base concentration factor	1.012	5/22/2018 1:35:32 PM	C:\Sirius_T3\KOH18D10.t3r
Acid concentration factor	0.998	5/22/2018 1:35:32 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Software version	1.1.3.0		
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	5/15/2018 2:12:22 PM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	3-22-18	5/15/2018 2:12:48 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3-22-18	5/15/2018 2:12:34 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	2-8-18	5/15/2018 2:14:14 PM
Port B	Cyclohexane		4/10/2018 8:40:51 AM
Port C	MeCN (50%, 0.15 M KCl)	4-16-18	5/15/2018 2:14:20 PM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	5/15/2018 2:12:54 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	1-31-2018	4/9/2018 9:14:11 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-11.54 mV		5/22/2018 1:35:56 PM
Filling solution	3M KCl	KCL095	5/21/2018 8:57:01 AM
Liquids			
Wash 1	50% IPA:50% Water		5/22/2018 8:38:15 AM
Wash 2	0.5% Trition X-100 in H20		5/22/2018 8:38:18 AM
Buffer position 1	pH7 Wash		5/22/2018 8:38:22 AM
Buffer position 2	pH 7		5/22/2018 8:38:25 AM
Storage position			5/22/2018 8:38:32 AM
Wash water	3.3e+003 mL	5-15-18	5/15/2018 2:11:48 PM
Waste	7.1e+003 mL		3/19/2018 10:48:12 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	897:26:49		11/23/2010 12:22:28 PM
Calibrated on	5/21/2018 2:44:22 PM		
Integration time	19		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location B3

UV-metric psKa_0417936-0002 Titration 1 of 3 18E-22013 Points 4 to 43

Results

pKa 1 **4.76**
pKa 2 **9.11**
RMSD **0.037 0.030 0.024**

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Results (continued)

Chi squared	**0.1583**
PCA calculated number of pKas	**4**
Average ionic strength	**0.158 M**
Average temperature	**25.0°C**
Analyte concentration range	**60.6 µM to 56.8 µM**
Methanol weight %	**48.9 %**
Dielectric constant	**56.9**
Water concentration	**25.0 M**
Number of pKas source	**Predicted**
Wavelength clipping	**230.0 nm to 450.0 nm**
pH clipping	**1.458 to 12.540**

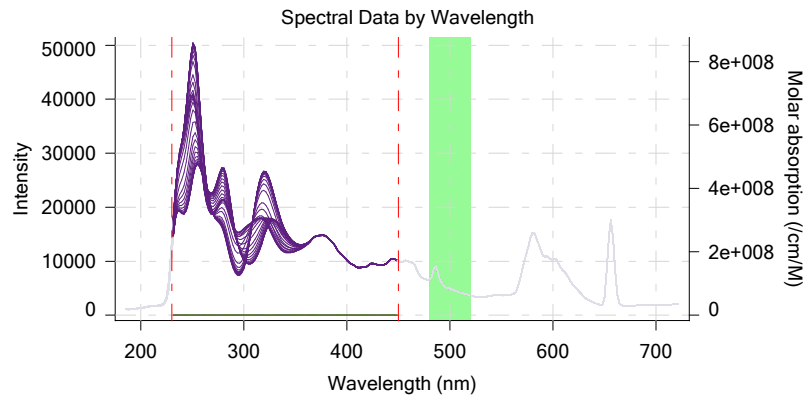
Warnings and errors

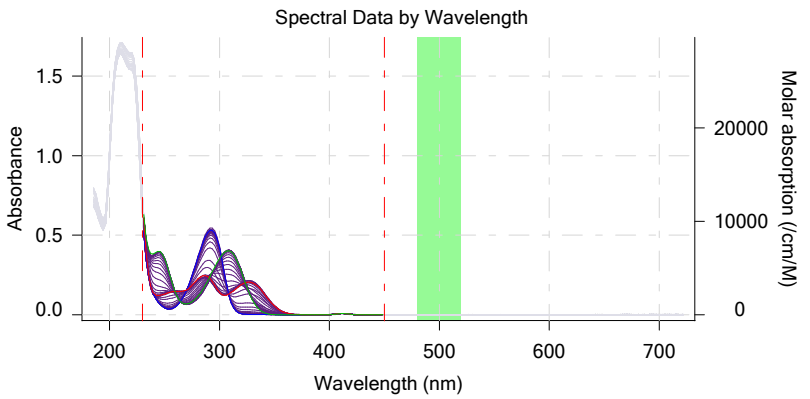
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

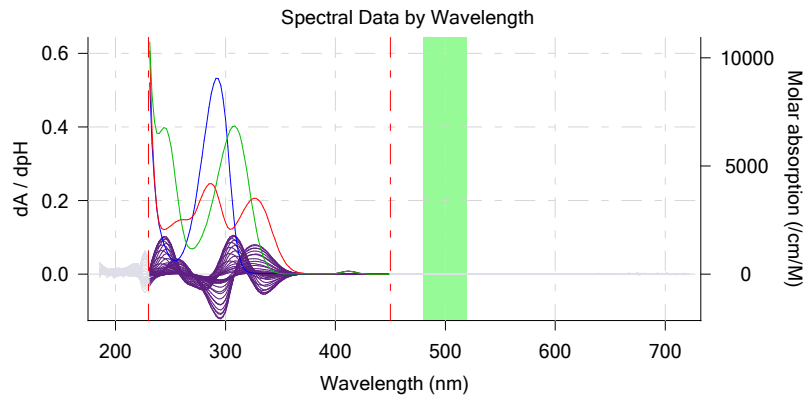
Assay Settings

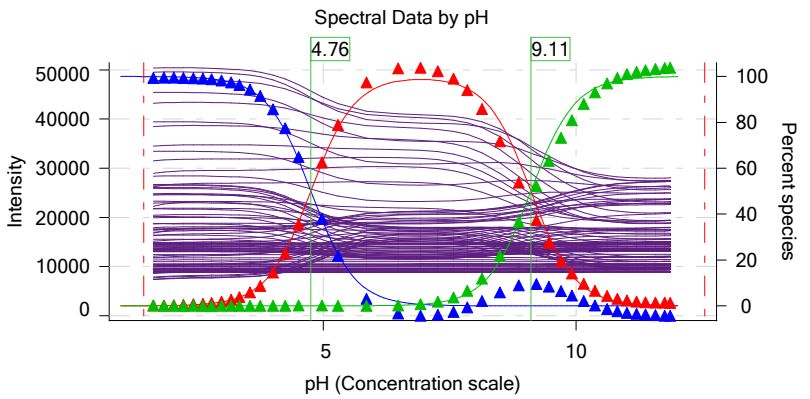
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs



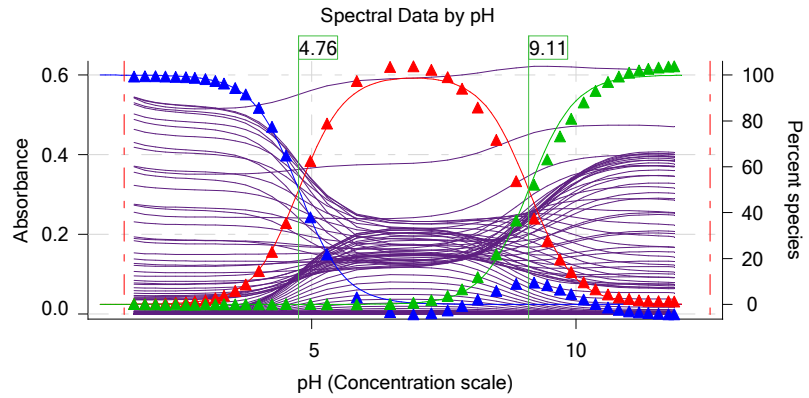


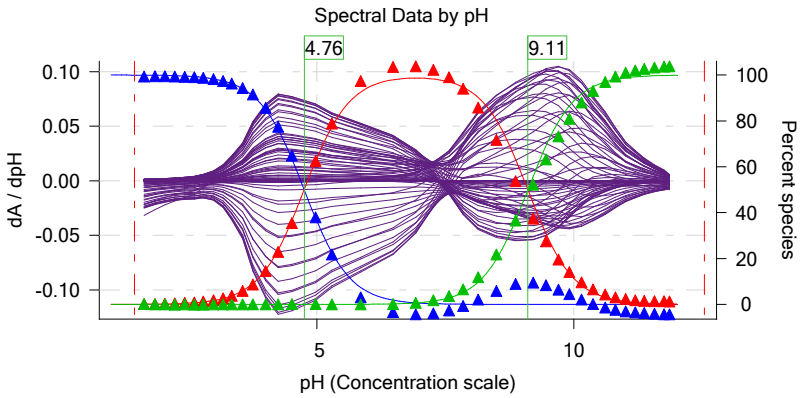


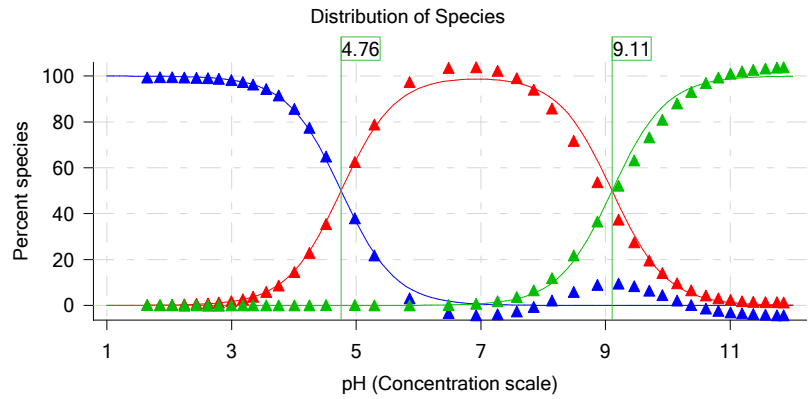


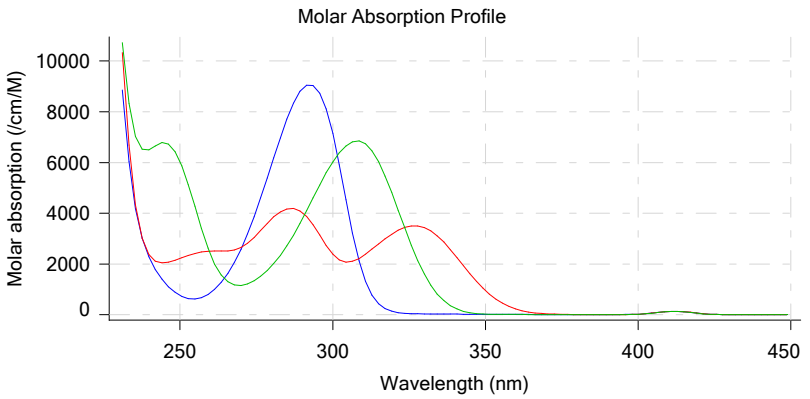
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

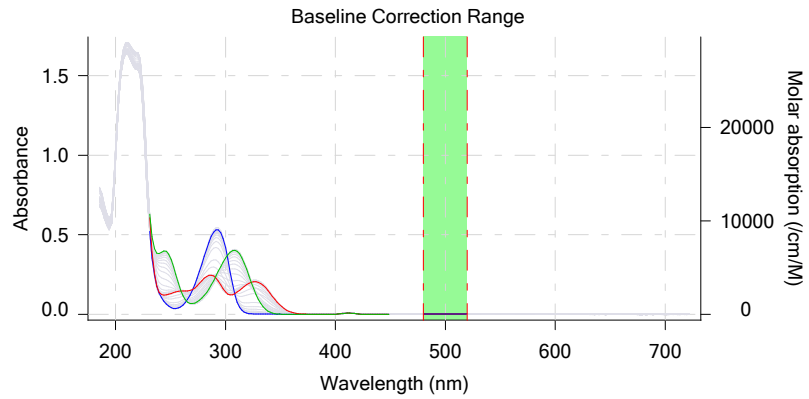
Graphs (continued)

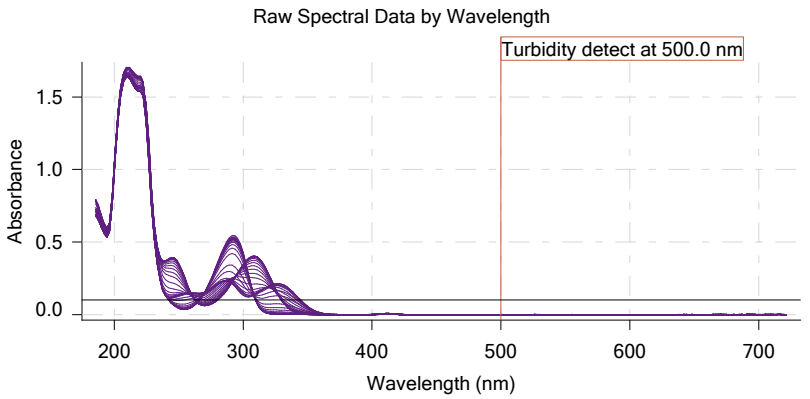












UV-metric psKa_0417936-0002 Titration 2 of 3 18E-22013 Points 45 to 85

Results

pKa 1	**4.79**
pKa 2	**9.03**
RMSD	**0.041 0.031 0.029**
Chi squared	**0.2196**
PCA calculated number of pKas	**3**
Average ionic strength	**0.168 M**
Average temperature	**25.0°C**
Analyte concentration range	**49.2 µM to 46.2 µM**
Methanol weight %	**39.0 %**
Dielectric constant	**61.4**
Water concentration	**30.6 M**

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.475 to 12.537**

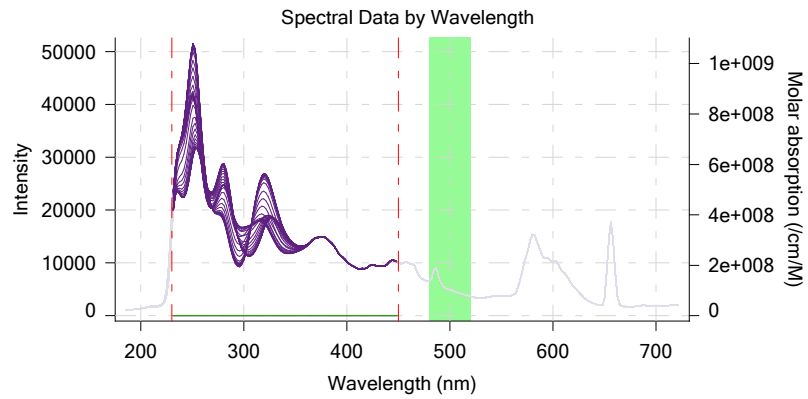
Warnings and errors

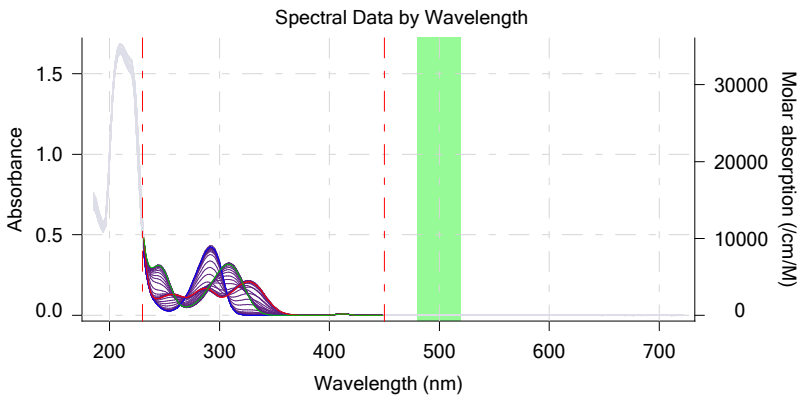
Errors None
Warnings PCA calculation disagrees with predicted number of pKas

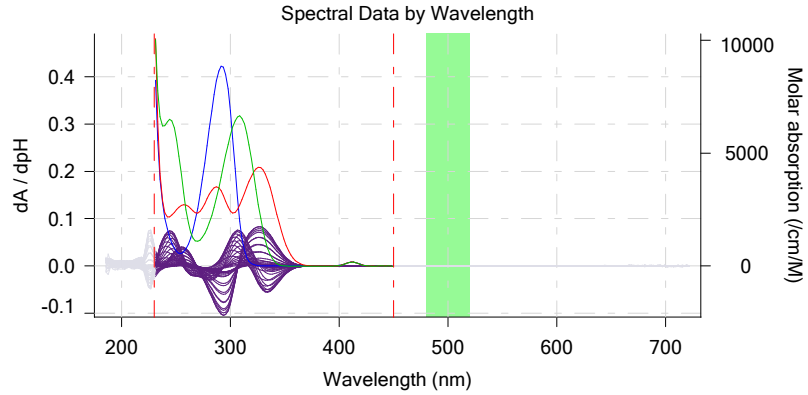
Assay Settings

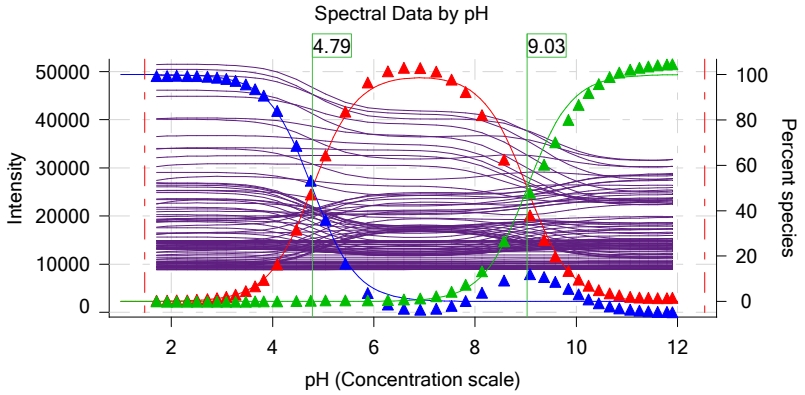
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs



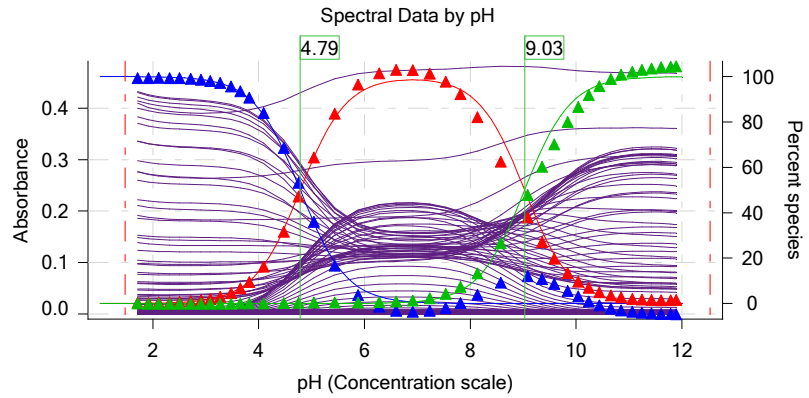


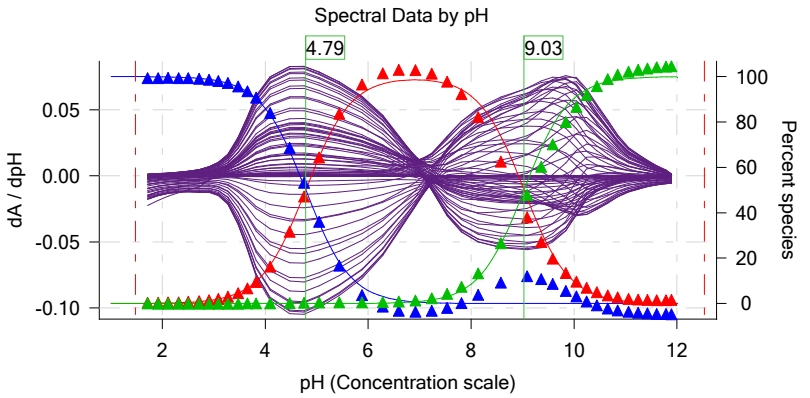


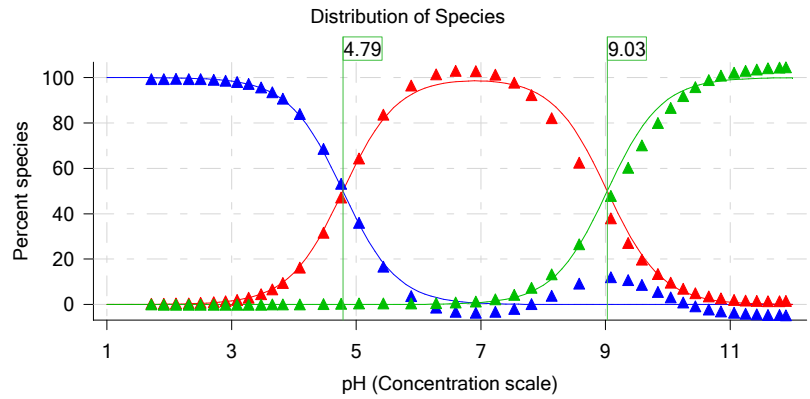


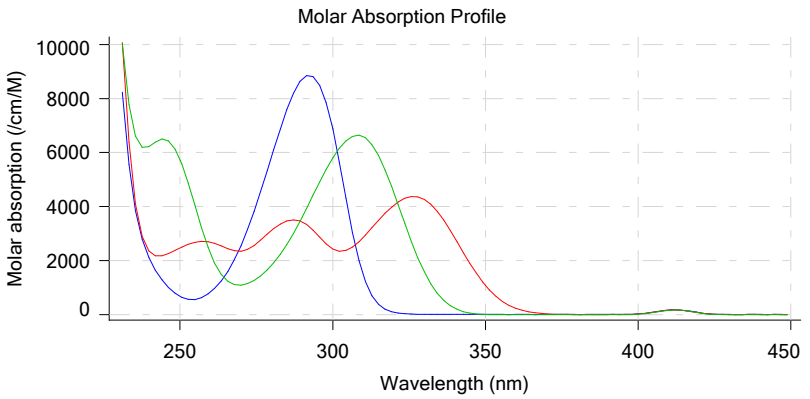
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

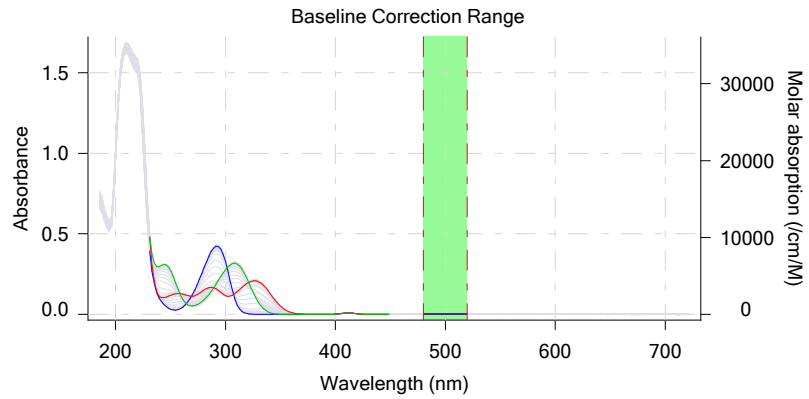
Graphs (continued)

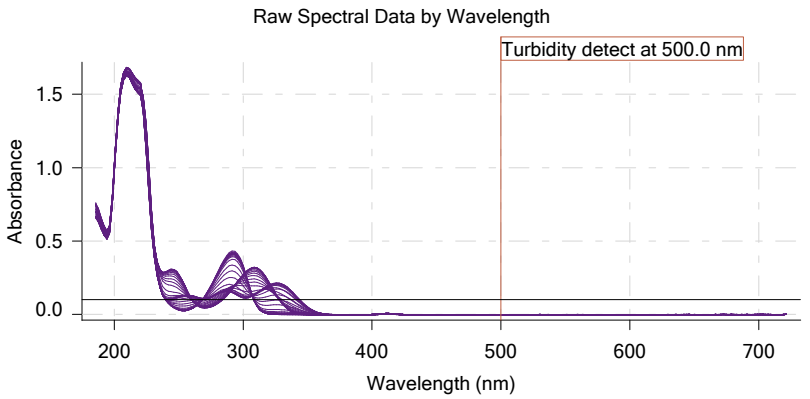












UV-metric psKa_0417936-0002 Titration 3 of 3 18E-22013 Points 87 to 120

Results

pKa 1	**4.82**
pKa 2	**8.95**
RMSD	**0.040 0.023 0.034**
Chi squared	**0.2385**
PCA calculated number of pKas	**2**
Average ionic strength	**0.175 M**
Average temperature	**25.0°C**
Analyte concentration range	**37.7 µM to 35.4 µM**
Methanol weight %	**29.3 %**
Dielectric constant	**65.8**
Water concentration	**36.3 M**

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Results (continued)

Number of pKas source **Predicted**
Wavelength clipping **230.0 nm to 450.0 nm**
pH clipping **1.497 to 12.523**

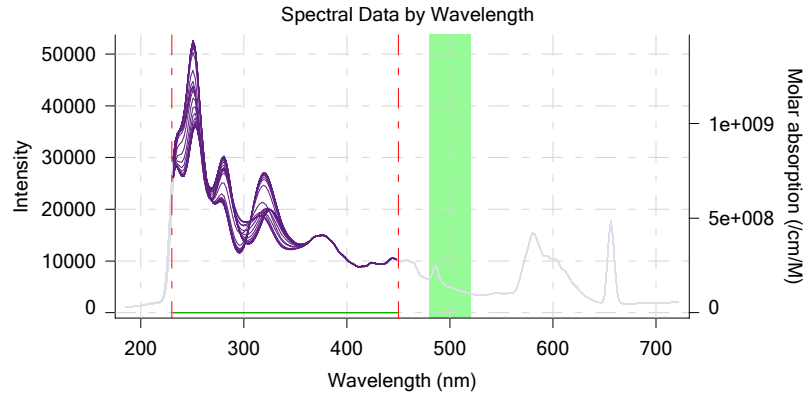
Warnings and errors

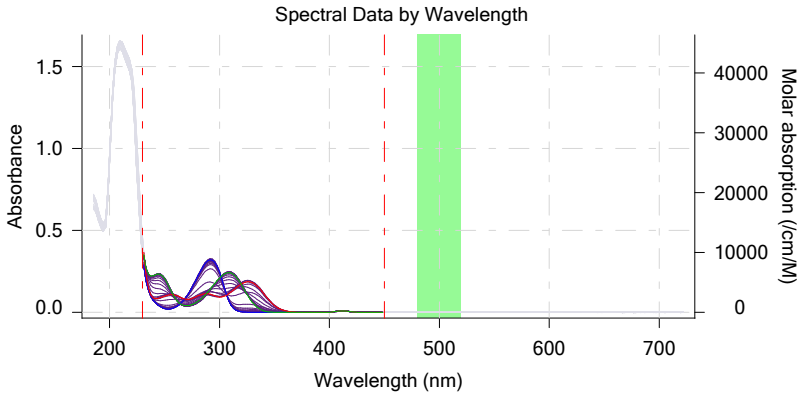
Errors None
Warnings None

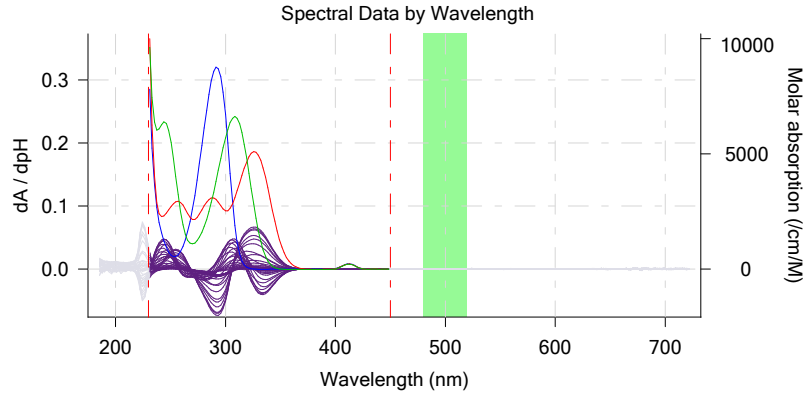
Assay Settings

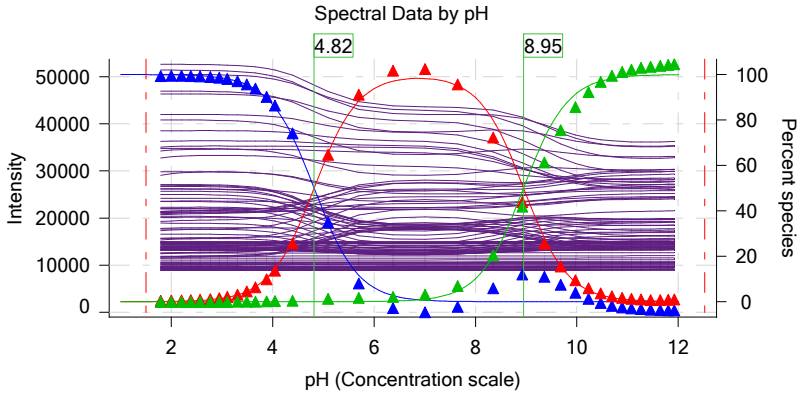
Setting	Value	Original Value	Date/Time changed	Imported from
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Assay Medium				
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			

Graphs



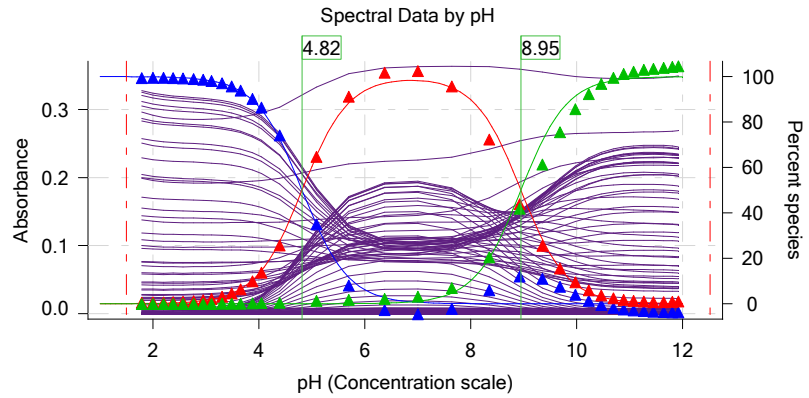


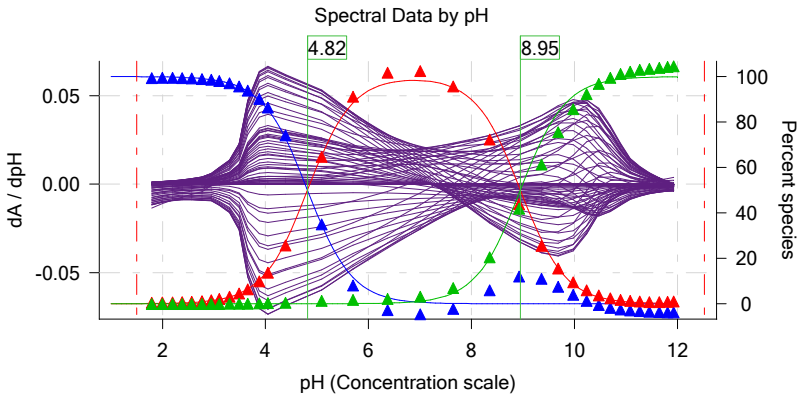


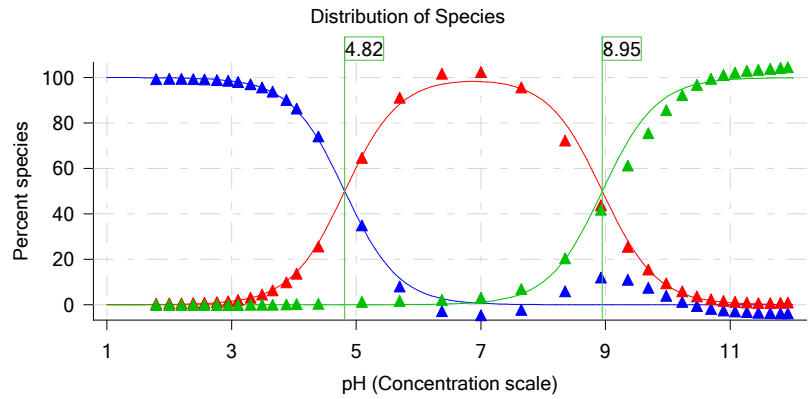


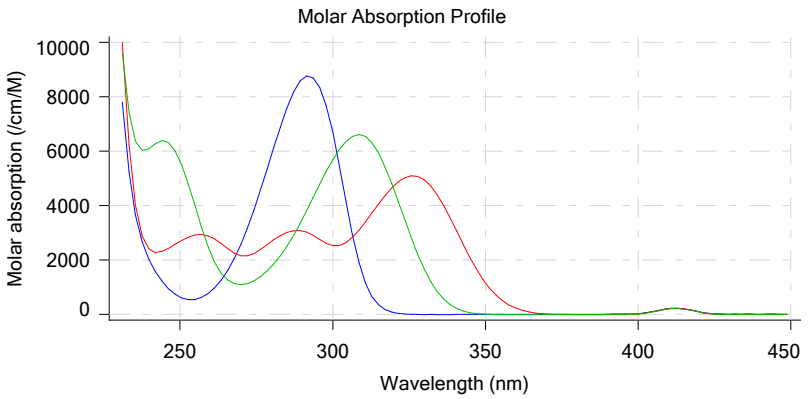
Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

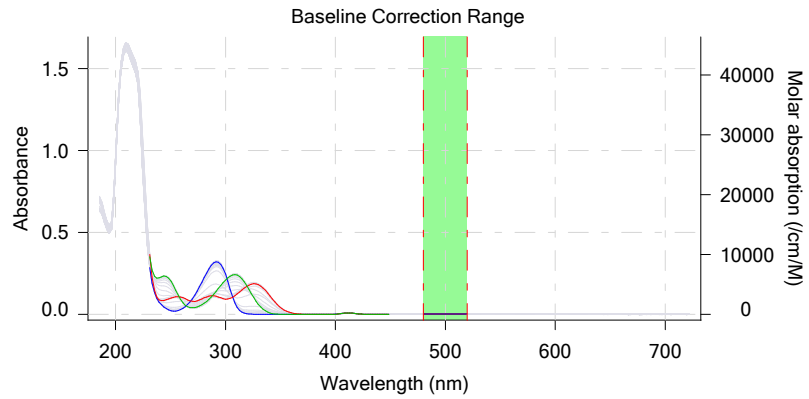
Graphs (continued)

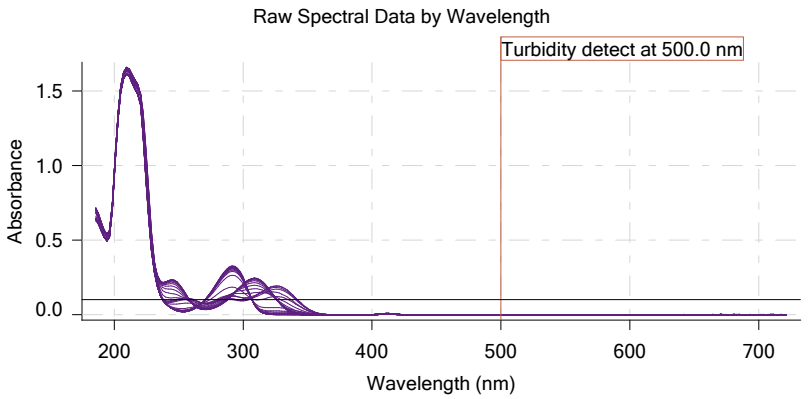












UV-metric psKa_0417936-0002 18E-22013 Assay 3 of 3

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	Pyridoxine HCl	5/22/2018 9:07:27 AM	User entered value
Sample by	Volume		Default value
Sample volume	0.0020 mL	5/22/2018 9:07:27 AM	User entered value
Solvent	DMSO		Default value
Sample concentration	0.048630 M	5/22/2018 9:07:27 AM	User entered value
Solubility	Unknown		Default value
Molecular weight	205.64	5/22/2018 9:07:35 AM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	5/22/2018 9:07:27 AM	User entered value
Sample is a	Ampholyte	5/22/2018 9:07:27 AM	User entered value
pKa 1	4.90	5/22/2018 9:07:27 AM	User entered value
Type	Base	5/22/2018 9:07:27 AM	User entered value

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
pKa 2	8.80	5/22/2018 9:07:27 AM	User entered value
Type	Acid	5/22/2018 9:07:27 AM	User entered value
logp (XH2 +)	-10.00		Default value
logP (neutral XH)	-10.00	5/22/2018 9:07:27 AM	User entered value
logP (X -)	-10.00		Default value
Stoichiometry	1.00000		Default value
Aprotic counterion name	Chloride		From standards.xml file
Stoichiometry	1.00		From standards.xml file
Charge per counterion	-1		From standards.xml file

Events

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squar
3:47.5	Dark spectrum								
3:48.9	Reference spectrum								
4:16.6	Volume reset due to vial change								
5:00.8	Initial pH = 7.80								
6:14.0	Data point 4	0.34995 mL	0.07707 mL	0.00000 mL	1.15005 mL	0.02500 mL	1.958	-0.00675	0.36684
6:43.0	Data point 5	0.34995 mL	0.07707 mL	0.02787 mL	1.15005 mL	0.02500 mL	2.159	0.01880	0.73494
7:00.1	Data point 6	0.34995 mL	0.07707 mL	0.04473 mL	1.15005 mL	0.02500 mL	2.350	0.02418	0.81115
7:17.0	Data point 7	0.34995 mL	0.07707 mL	0.05543 mL	1.15005 mL	0.02500 mL	2.538	0.00766	0.48680
7:33.8	Data point 8	0.34995 mL	0.07707 mL	0.06251 mL	1.15005 mL	0.02500 mL	2.729	0.00940	0.69522
7:50.7	Data point 9	0.34995 mL	0.07707 mL	0.06698 mL	1.15005 mL	0.02500 mL	2.915	0.02148	0.94661
8:07.5	Data point 10	0.34995 mL	0.07707 mL	0.06987 mL	1.15005 mL	0.02500 mL	3.083	0.01310	0.92140
8:39.8	Data point 11	0.34995 mL	0.07707 mL	0.07180 mL	1.15005 mL	0.02500 mL	3.282	0.01748	0.95225
8:56.5	Data point 12	0.34995 mL	0.07707 mL	0.07305 mL	1.15005 mL	0.02500 mL	3.467	0.02450	0.97126
9:13.3	Data point 13	0.34995 mL	0.07707 mL	0.07385 mL	1.15005 mL	0.02500 mL	3.630	0.02600	0.98283
9:45.5	Data point 14	0.34995 mL	0.07707 mL	0.07462 mL	1.15005 mL	0.02500 mL	3.838	0.03686	0.95342
10:12.5	Data point 15	0.34995 mL	0.07707 mL	0.07502 mL	1.15005 mL	0.02500 mL	4.034	0.04323	0.92672
10:34.4	Data point 16	0.34995 mL	0.07707 mL	0.07538 mL	1.15005 mL	0.02500 mL	4.283	0.09629	0.99054
11:01.3	Data point 17	0.34995 mL	0.07707 mL	0.07563 mL	1.15005 mL	0.02500 mL	4.523	0.09939	0.99587
11:37.7	Data point 18	0.34995 mL	0.07707 mL	0.07589 mL	1.15005 mL	0.02500 mL	4.787	0.10033	0.99639
12:27.5	Data point 19	0.34995 mL	0.07707 mL	0.07627 mL	1.15005 mL	0.02500 mL	5.242	0.09340	0.95236
13:19.0	Data point 20	0.34995 mL	0.07707 mL	0.07639 mL	1.15005 mL	0.02500 mL	5.554	-0.06084	0.38499
13:54.7	Data point 21	0.34995 mL	0.07707 mL	0.07648 mL	1.15005 mL	0.02500 mL	6.113	0.12647	0.99662
15:11.6	Data point 22	0.34995 mL	0.07707 mL	0.07665 mL	1.15005 mL	0.02500 mL	6.733	0.09975	0.98674
16:16.1	Data point 23	0.34995 mL	0.07707 mL	0.07676 mL	1.15005 mL	0.02500 mL	7.168	0.09998	0.99022
17:12.6	Data point 24	0.34995 mL	0.07707 mL	0.07691 mL	1.15005 mL	0.02500 mL	7.505	0.10061	0.99032
17:59.0	Data point 25	0.34995 mL	0.07707 mL	0.07707 mL	1.15005 mL	0.02500 mL	7.810	0.09931	0.99002
18:44.0	Data point 26	0.34995 mL	0.07707 mL	0.07721 mL	1.15005 mL	0.02500 mL	8.082	0.09998	0.99187
19:28.4	Data point 27	0.34995 mL	0.07707 mL	0.07735 mL	1.15005 mL	0.02500 mL	8.371	0.09979	0.99259
20:08.2	Data point 28	0.34995 mL	0.07707 mL	0.07749 mL	1.15005 mL	0.02500 mL	8.718	0.09893	0.98482
20:58.7	Data point 29	0.34995 mL	0.07707 mL	0.07763 mL	1.15005 mL	0.02500 mL	9.090	0.09803	0.98111
21:40.6	Data point 30	0.34995 mL	0.07707 mL	0.07778 mL	1.15005 mL	0.02500 mL	9.429	0.09614	0.98682
22:21.0	Data point 31	0.34995 mL	0.07707 mL	0.07789 mL	1.15005 mL	0.02500 mL	9.673	0.10014	0.98157
22:54.0	Data point 32	0.34995 mL	0.07707 mL	0.07806 mL	1.15005 mL	0.02500 mL	9.914	0.09602	0.97678
23:22.1	Data point 33	0.34995 mL	0.07707 mL	0.07825 mL	1.15005 mL	0.02500 mL	10.124	0.07182	0.97071
23:43.8	Data point 34	0.34995 mL	0.07707 mL	0.07848 mL	1.15005 mL	0.02500 mL	10.357	0.04495	0.97842
24:00.5	Data point 35	0.34995 mL	0.07707 mL	0.07881 mL	1.15005 mL	0.02500 mL	10.577	0.01818	0.89241
24:17.0	Data point 36	0.34995 mL	0.07707 mL	0.07937 mL	1.15005 mL	0.02500 mL	10.811	0.00997	0.86656
24:49.1	Data point 37	0.34995 mL	0.07707 mL	0.08034 mL	1.15005 mL	0.02500 mL	11.010	0.00553	0.83760
25:05.8	Data point 38	0.34995 mL	0.07707 mL	0.08184 mL	1.15005 mL	0.02500 mL	11.201	0.00397	0.60445
25:22.5	Data point 39	0.34995 mL	0.07707 mL	0.08415 mL	1.15005 mL	0.02500 mL	11.387	0.00407	0.49542
25:39.2	Data point 40	0.34995 mL	0.07707 mL	0.08772 mL	1.15005 mL	0.02500 mL	11.562	0.00038	0.00606
25:56.0	Data point 41	0.34995 mL	0.07707 mL	0.09309 mL	1.15005 mL	0.02500 mL	11.754	-0.00112	0.03530
26:12.8	Data point 42	0.34995 mL	0.07707 mL	0.10153 mL	1.15005 mL	0.02500 mL	11.936	0.00241	0.18901
26:29.7	Data point 43	0.34995 mL	0.07707 mL	0.10823 mL	1.15005 mL	0.02500 mL	12.040	0.00108	0.05931
28:11.9	Reference spectrum								

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
29:16.3	Data point 45	0.50000 mL	0.19099 mL	0.10826 mL	1.15005 mL	0.02500 mL	1.975	-0.09545	0.97685	0.00
29:46.1	Data point 46	0.50000 mL	0.19099 mL	0.13972 mL	1.15005 mL	0.02500 mL	2.171	0.00276	0.19246	0.00
30:03.2	Data point 47	0.50000 mL	0.19099 mL	0.15774 mL	1.15005 mL	0.02500 mL	2.361	0.01031	0.65796	0.00
30:20.1	Data point 48	0.50000 mL	0.19099 mL	0.16924 mL	1.15005 mL	0.02500 mL	2.562	0.00698	0.48137	0.00
30:36.9	Data point 49	0.50000 mL	0.19099 mL	0.17648 mL	1.15005 mL	0.02500 mL	2.749	0.00669	0.30673	0.00
30:53.8	Data point 50	0.50000 mL	0.19099 mL	0.18116 mL	1.15005 mL	0.02500 mL	2.955	0.01364	0.63909	0.00
31:10.5	Data point 51	0.50000 mL	0.19099 mL	0.18403 mL	1.15005 mL	0.02500 mL	3.145	0.02412	0.95389	0.00
31:27.3	Data point 52	0.50000 mL	0.19099 mL	0.18589 mL	1.15005 mL	0.02500 mL	3.323	0.03326	0.97931	0.00
31:44.1	Data point 53	0.50000 mL	0.19099 mL	0.18711 mL	1.15005 mL	0.02500 mL	3.506	0.03190	0.96348	0.00
32:00.8	Data point 54	0.50000 mL	0.19099 mL	0.18791 mL	1.15005 mL	0.02500 mL	3.707	0.03611	0.93670	0.00
32:17.4	Data point 55	0.50000 mL	0.19099 mL	0.18840 mL	1.15005 mL	0.02500 mL	3.886	0.03880	0.93500	0.00
32:34.1	Data point 56	0.50000 mL	0.19099 mL	0.18874 mL	1.15005 mL	0.02500 mL	4.052	0.06475	0.96862	0.00
32:55.8	Data point 57	0.50000 mL	0.19099 mL	0.18906 mL	1.15005 mL	0.02500 mL	4.321	0.09564	0.95362	0.00
33:18.2	Data point 58	0.50000 mL	0.19099 mL	0.18932 mL	1.15005 mL	0.02500 mL	4.695	0.09928	0.97259	0.00
33:53.7	Data point 59	0.50000 mL	0.19099 mL	0.18949 mL	1.15005 mL	0.02500 mL	4.975	0.09964	0.97032	0.00
34:22.9	Data point 60	0.50000 mL	0.19099 mL	0.18958 mL	1.15005 mL	0.02500 mL	5.260	0.09819	0.98682	0.00
34:59.2	Data point 61	0.50000 mL	0.19099 mL	0.18968 mL	1.15005 mL	0.02500 mL	5.649	0.09975	0.98785	0.00
35:47.6	Data point 62	0.50000 mL	0.19099 mL	0.18977 mL	1.15005 mL	0.02500 mL	6.090	0.09839	0.98247	0.00
36:34.4	Data point 63	0.50000 mL	0.19099 mL	0.18986 mL	1.15005 mL	0.02500 mL	6.486	0.09922	0.98693	0.00
37:20.3	Data point 64	0.50000 mL	0.19099 mL	0.18996 mL	1.15005 mL	0.02500 mL	6.799	0.10084	0.99471	0.00
38:01.1	Data point 65	0.50000 mL	0.19099 mL	0.19007 mL	1.15005 mL	0.02500 mL	7.115	0.09758	0.98427	0.00
38:43.0	Data point 66	0.50000 mL	0.19099 mL	0.19022 mL	1.15005 mL	0.02500 mL	7.428	0.09730	0.98030	0.00
39:18.4	Data point 67	0.50000 mL	0.19099 mL	0.19036 mL	1.15005 mL	0.02500 mL	7.727	0.09850	0.96000	0.00
39:57.4	Data point 68	0.50000 mL	0.19099 mL	0.19050 mL	1.15005 mL	0.02500 mL	8.004	0.09320	0.98471	0.00
40:38.8	Data point 69	0.50000 mL	0.19099 mL	0.19064 mL	1.15005 mL	0.02500 mL	8.324	0.09529	0.97727	0.00
41:17.8	Data point 70	0.50000 mL	0.19099 mL	0.19080 mL	1.15005 mL	0.02500 mL	8.758	0.09647	0.96427	0.00
41:57.2	Data point 71	0.50000 mL	0.19099 mL	0.19102 mL	1.15005 mL	0.02500 mL	9.264	0.09505	0.96325	0.00
42:30.6	Data point 72	0.50000 mL	0.19099 mL	0.19120 mL	1.15005 mL	0.02500 mL	9.535	0.09099	0.94785	0.00
43:00.5	Data point 73	0.50000 mL	0.19099 mL	0.19139 mL	1.15005 mL	0.02500 mL	9.758	0.09689	0.92452	0.00
43:22.7	Data point 74	0.50000 mL	0.19099 mL	0.19165 mL	1.15005 mL	0.02500 mL	10.010	0.05681	0.89973	0.00
43:44.5	Data point 75	0.50000 mL	0.19099 mL	0.19198 mL	1.15005 mL	0.02500 mL	10.212	0.02831	0.87650	0.00
44:16.5	Data point 76	0.50000 mL	0.19099 mL	0.19250 mL	1.15005 mL	0.02500 mL	10.409	0.03374	0.88383	0.00
44:48.6	Data point 77	0.50000 mL	0.19099 mL	0.19323 mL	1.15005 mL	0.02500 mL	10.606	0.01230	0.77321	0.00
45:15.6	Data point 78	0.50000 mL	0.19099 mL	0.19452 mL	1.15005 mL	0.02500 mL	10.818	0.00729	0.82566	0.00
45:42.6	Data point 79	0.50000 mL	0.19099 mL	0.19603 mL	1.15005 mL	0.02500 mL	11.010	0.00079	0.02605	0.00
45:59.4	Data point 80	0.50000 mL	0.19099 mL	0.19812 mL	1.15005 mL	0.02500 mL	11.218	0.00065	0.02108	0.00
46:16.2	Data point 81	0.50000 mL	0.19099 mL	0.20150 mL	1.15005 mL	0.02500 mL	11.399	-0.00077	0.03197	0.00
46:33.1	Data point 82	0.50000 mL	0.19099 mL	0.20666 mL	1.15005 mL	0.02500 mL	11.578	0.00407	0.41820	0.00
46:50.0	Data point 83	0.50000 mL	0.19099 mL	0.21449 mL	1.15005 mL	0.02500 mL	11.754	0.00080	0.04674	0.00
47:07.0	Data point 84	0.50000 mL	0.19099 mL	0.22636 mL	1.15005 mL	0.02500 mL	11.934	0.00185	0.12773	0.00
47:23.9	Data point 85	0.50000 mL	0.19099 mL	0.23594 mL	1.15005 mL	0.02500 mL	12.037	0.00236	0.21950	0.00
49:25.3	Reference spectrum									
50:33.5	Data point 87	0.83996 mL	0.32858 mL	0.23596 mL	1.15005 mL	0.02500 mL	1.997	-0.09665	0.98013	0.00
51:17.1	Data point 88	0.83996 mL	0.32858 mL	0.27225 mL	1.15005 mL	0.02500 mL	2.198	-0.00138	0.06588	0.00
51:44.6	Data point 89	0.83996 mL	0.32858 mL	0.29231 mL	1.15005 mL	0.02500 mL	2.393	0.00349	0.09831	0.00
52:01.6	Data point 90	0.83996 mL	0.32858 mL	0.30456 mL	1.15005 mL	0.02500 mL	2.576	-0.02010	0.83036	0.00
52:18.6	Data point 91	0.83996 mL	0.32858 mL	0.31268 mL	1.15005 mL	0.02500 mL	2.756	-0.02760	0.83347	0.00
52:35.4	Data point 92	0.83996 mL	0.32858 mL	0.31801 mL	1.15005 mL	0.02500 mL	2.954	0.02357	0.77780	0.00
52:52.2	Data point 93	0.83996 mL	0.32858 mL	0.32133 mL	1.15005 mL	0.02500 mL	3.132	0.00080	0.02816	0.00
53:08.9	Data point 94	0.83996 mL	0.32858 mL	0.32356 mL	1.15005 mL	0.02500 mL	3.288	0.01078	0.80012	0.00
53:35.9	Data point 95	0.83996 mL	0.32858 mL	0.32502 mL	1.15005 mL	0.02500 mL	3.486	0.02594	0.98050	0.00
53:52.6	Data point 96	0.83996 mL	0.32858 mL	0.32599 mL	1.15005 mL	0.02500 mL	3.669	0.02302	0.90868	0.00
54:09.2	Data point 97	0.83996 mL	0.32858 mL	0.32662 mL	1.15005 mL	0.02500 mL	3.835	0.03133	0.98006	0.00
54:31.0	Data point 98	0.83996 mL	0.32858 mL	0.32712 mL	1.15005 mL	0.02500 mL	4.053	0.09511	0.99496	0.00
54:47.7	Data point 99	0.83996 mL	0.32858 mL	0.32738 mL	1.15005 mL	0.02500 mL	4.221	0.09919	0.98807	0.00
55:32.0	Data point 100	0.83996 mL	0.32858 mL	0.32773 mL	1.15005 mL	0.02500 mL	4.563	0.09992	0.98994	0.00
56:15.6	Data point 101	0.83996 mL	0.32858 mL	0.32815 mL	1.15005 mL	0.02500 mL	5.255	0.09800	0.98954	0.00
57:07.0	Data point 102	0.83996 mL	0.32858 mL	0.32836 mL	1.15005 mL	0.02500 mL	5.858	0.09893	0.99333	0.00

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Events (continued)

Time	Event	Water	Acid	Base	Methanol	Buffer	pH	dpH/dt	pH R-squared	pH SD
58:12.4	Data point 103	0.83996 mL	0.32858 mL	0.32867 mL	1.15005 mL	0.02500 mL	6.528	0.08309	0.76810	0.0046
58:42.8	Data point 104	0.83996 mL	0.32858 mL	0.32898 mL	1.15005 mL	0.02500 mL	7.152	0.06530	0.59596	0.0041
59:16.2	Data point 105	0.83996 mL	0.32858 mL	0.32935 mL	1.15005 mL	0.02500 mL	7.790	0.09756	0.98263	0.0048
59:56.6	Data point 106	0.83996 mL	0.32858 mL	0.32966 mL	1.15005 mL	0.02500 mL	8.488	0.09740	0.97254	0.0048
1:00:49.8	Data point 107	0.83996 mL	0.32858 mL	0.32999 mL	1.15005 mL	0.02500 mL	9.057	0.09636	0.98563	0.0047
1:01:37.7	Data point 108	0.83996 mL	0.32858 mL	0.33034 mL	1.15005 mL	0.02500 mL	9.486	0.09860	0.97841	0.0049
1:02:10.7	Data point 109	0.83996 mL	0.32858 mL	0.33100 mL	1.15005 mL	0.02500 mL	9.811	0.10007	0.99467	0.0049
1:02:38.7	Data point 110	0.83996 mL	0.32858 mL	0.33175 mL	1.15005 mL	0.02500 mL	10.098	0.06725	0.93744	0.0034
1:03:00.6	Data point 111	0.83996 mL	0.32858 mL	0.33248 mL	1.15005 mL	0.02500 mL	10.353	0.02323	0.91021	0.0012
1:03:32.7	Data point 112	0.83996 mL	0.32858 mL	0.33354 mL	1.15005 mL	0.02500 mL	10.588	0.01887	0.91930	0.0009
1:04:04.9	Data point 113	0.83996 mL	0.32858 mL	0.33481 mL	1.15005 mL	0.02500 mL	10.811	0.00541	0.59517	0.0003
1:04:21.6	Data point 114	0.83996 mL	0.32858 mL	0.33683 mL	1.15005 mL	0.02500 mL	11.007	-0.01169	0.83876	0.0006
1:04:38.2	Data point 115	0.83996 mL	0.32858 mL	0.34001 mL	1.15005 mL	0.02500 mL	11.191	-0.01953	0.88709	0.0010
1:04:55.1	Data point 116	0.83996 mL	0.32858 mL	0.34485 mL	1.15005 mL	0.02500 mL	11.379	-0.01258	0.84686	0.0006
1:05:12.0	Data point 117	0.83996 mL	0.32858 mL	0.35237 mL	1.15005 mL	0.02500 mL	11.562	-0.00673	0.47279	0.0004
1:05:29.0	Data point 118	0.83996 mL	0.32858 mL	0.36395 mL	1.15005 mL	0.02500 mL	11.749	-0.01133	0.90688	0.0005
1:05:46.1	Data point 119	0.83996 mL	0.32858 mL	0.38208 mL	1.15005 mL	0.02500 mL	11.906	-0.00971	0.51929	0.0006
1:06:08.4	Data point 120	0.83996 mL	0.32858 mL	0.39866 mL	1.15005 mL	0.02500 mL	12.023	-0.00268	0.19720	0.0003
1:08:13.7	Assay volumes	1.08996 mL	0.49266 mL	0.39866 mL	1.15005 mL	0.02500 mL				

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Separate reference vial	Yes			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	12.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	Spectrometer			
Monitor at a wavelength of	500.0 nm			
Absorbance threshold of	0.100			
Collect turbidity sensor data	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	15%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
Cosolvent in use	Yes			
Cosolvent type	Methanol			
Cosolvent volume	1.15 mL			
Cosolvent added	Automatic			
ISA water volume	0.35 mL			
Water added	Automatic			
After water addition, stir for	5 seconds			
At a speed of	15%			
Buffer in use	Yes			
Buffer type	Phosphate Buffer			
Volume of buffer introduced	0.025000 mL			
Add buffer manually	Manual			
After medium addition, stir for	5 seconds			
Sample Sonication				

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Sonicate	No			
Sample Dissolution				
Perform a dissolution stage	No			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	15%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	10 seconds			
Titration 2				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.15 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Titration 3				
Titrate from	Low to high pH			
Additional cosolvent volume	0.00 mL			
Add additional water	0.34 mL			
Additional water added	Automatic			
After pH adjust stir for	10 seconds			
Data Point Stability				
Stir during data point collection	Yes			
For point collection, stir at	15%			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00500 dpH/dt			
Stability timeout after	60 seconds			
Experiment cleanup				
Adjust pH to cleanup	To start pH			
And then stir for	60 seconds			
For cleaning, stir at	20%			
Then add water volume	0.25 mL			
And then stir for	30 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.144	5/22/2018 2:50:50 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus S	0.9948	5/22/2018 2:50:50 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jH	1.0	5/22/2018 2:50:50 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Four-Plus jOH	-0.8	5/22/2018 2:50:50 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r
Base concentration factor	1.012	5/22/2018 2:50:50 PM	C:\Sirius_T3\KOH18D10.t3r
Acid concentration factor	0.998	5/22/2018 2:50:50 PM	C:\Sirius_T3\18E-22009_Blank standardisation.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T311053		
Instrument type	T3 Simulator		
Software version	1.1.3.0		

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Dispenser module		T3DM1100253	3/31/2009 6:24:52 AM
Dispenser 0	Water		3/31/2009 6:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	2-6-18	5/15/2018 2:12:22 PM
Dispenser 2	Acid		3/31/2009 6:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	3-22-18	5/15/2018 2:12:48 PM
Dispenser 1	Base		3/31/2009 6:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	3-22-18	5/15/2018 2:12:34 PM
Dispenser 5	Cosolvent		3/31/2009 6:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 6:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	2-8-18	5/15/2018 2:14:14 PM
Port B	Cyclohexane		4/10/2018 8:40:51 AM
Port C	MeCN (50%, 0.15 M KCl)	4-16-18	5/15/2018 2:14:20 PM
Dispenser 3	Buffer		8/3/2010 6:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	1-31-2018	5/15/2018 2:12:54 PM
Dispenser 6	Octanol		10/22/2010 11:52:43 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	1-31-2018	4/9/2018 9:14:11 AM
Titrator		T3TM1100153	3/31/2009 6:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0769	8/15/2017 10:21:54 AM
E0 calibration	-12.44 mV		5/22/2018 2:51:14 PM
Filling solution	3M KCl	KCL095	5/21/2018 8:57:01 AM
Liquids			
Wash 1	50% IPA:50% Water		5/22/2018 8:38:15 AM
Wash 2	0.5% Trition X-100 in H20		5/22/2018 8:38:18 AM
Buffer position 1	pH7 Wash		5/22/2018 8:38:22 AM
Buffer position 2	pH 7		5/22/2018 8:38:25 AM
Storage position			5/22/2018 8:38:32 AM
Wash water	3.2e+003 mL	5-15-18	5/15/2018 2:11:48 PM
Waste	7.3e+003 mL		3/19/2018 10:48:12 AM
Temperature controller			8/5/2010 7:35:13 AM
Turbidity detector			3/31/2009 6:24:45 AM
Spectrometer		072390	11/23/2010 12:22:28 PM
Dip probe		11086	
Wavelength coefficient A0	185.563		
Wavelength coefficient A1	2.17439		
Wavelength coefficient A2	-0.000285622		
Total lamp lit time	897:26:49		11/23/2010 12:22:28 PM
Calibrated on	5/21/2018 2:44:22 PM		
Integration time	19		
Scans averaged	10		
Autoloader		T3AL1100237	11/10/2015 10:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		

Multiset name: **0417936-0002** Instrument ID: **T311053**
Analyst: **Dorothy Levorse**
Filename: **C:\Sirius_T3\Pyridoxine_HCl_UV_MeOH_05_22_18.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	Spectrometer	Spectrometer
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00
Exclude turbid points	Yes	Yes
Low intensity warning threshold	100	100
Minimum absorbance change threshold	0.100	0.100
Eigenvector autocorrelation threshold	0.80	0.80
Maximum RMSD severe warning	0.250	0.250
Maximum RMSD warning	0.050	0.050

Tray Information

Title
Location B5